Research Programme for Future Electronics

Project Reports

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Preface

The Research Programme for Future Electronics (TULE; 2003–2006) launched by the Academy of Finland has been an important step on the path of Academy support to high-level electronics and materials research. Its foregoers have been e.g. the Research Programme for Electronic Materials and Microsystems (EMMA; 1999–2002) and the Research Programme on Materials and Structure Research (MATRA; 1994–2000). Materials and electronics research programmatic funding is also continued in the present Research Programme on Nanoscience (FinNano; 2006–2010). It has been a sustainable strategy by the Academy to strengthen these nationally important research fields. The Academy's Research Council for Natural Sciences and Engineering must be separately mentioned here as the original proposer of the above programmes.

The TULE research programme originally had a total funding of 6.75 million euros and it consisted of 13 research projects. The programme steering committee decided, in two steps, to strengthen the programme with additional projects, and in the end there were 18 projects under the TULE umbrella with a total funding of 7.51 million euros. Programme cooperation at the national level was most active with the Miniaturizing Electronics Technology Programme (ELMO; 2002–2005) funded by Tekes – Finnish Funding Agency for Technology and Innovation. International cooperation was targeted at the ERA-NET project MATERA, a European network project for organisations funding the field of material science and technology.

This publication of the TULE programme is a collection of the research reports by the funded projects. The results show a great amount of scientific effort that is fully or partly funded by TULE: 61 PhD dissertations, over 430 refereed journal articles and more than 250 conference papers. Regarding application of results, it is observed that industrial projects and spin-off companies were mentioned by several projects. Adding other funding sources to the Academy's funding, the total funding volume of TULE research programme amounted to 11.7 million euros.

In light of these results, the main objectives of the programme, i.e. "to promote long-term and high-level basic research leading to new innovative applications, and to support the ongoing research and development effort within the Finnish electronics and electrical industry", can be considered to have been well achieved.

In addition to showing achievements within the framework of the TULE programme, the reports give an overall picture of the advancement and scientific level of electronics research in Finland.

Helsinki, February 2007

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CONSTRAINT-DRIVEN PLATFORM-BASED SYSTEM-ON-CHIP DESIGN

Jari Nurmi[1]

Abstract

Efficient platform-based design requires new methodologies to (1) model functional IPs and the communication platform itself, to (2) systematically proceed from an initial system specification to an architecture model composed of a platform model and a set of functional IP models, to (3) map the architecture model to actual concrete IP components in an optimal manner, and to (4) reliably verify, in a number of phases, both functional and timing correctness of the resulting system configuration. The purpose of the CONSTRAIN project was to address these crucial issues. Collaboration with University of Turku was carried out on unofficial basis since their part was not funded at all by the Academy. The collaboration also produced many joint publications where the credit was given to other projects with more balanced funding basis for cooperation. This includes one Kluwer book on Interconnect-Centric Design, which also falls into the scope of this project. The group at TUT made a review of arbitration and routing schemes for on-chip communication networks that was published as a book chapter. Also several other publications were made. The group is actively cooperating in Europe and worldwide, including EU projects, conference organization, and a variety of other activities. The research in this project focused mostly on eXtended Generalized Fat Tree (XGFT) interconnection network. Two adaptive routing algorithms in this network topology were evaluated and implemented to achieve the physical characteristics of the communication network. The properties of XGFT communications as reusable interconnect IP blocks were researched. Finally, fault tolerance and dynamic reconfigurability aspects have been introduced to this communication network. The fault tolerance and adaptability are increasingly important in future nanoscale System-on-Chip implementations, where the fault and error probabilities are increasing. In addition to XGFTs, the developed schemes are applicable to other network topologies such as Mesh and Full Mesh networks. The area overhead of the Fault Detection and Repair (FDAR) functionality is in the order of only 10-15%.

1 Partners and Funding

1.1 Institute of Digital and Computer Systems, Tampere University of Technology

The research group consists of project leader professor Jari Nurmi and senior researcher Heikki Kariniemi who carried out the project as a postgraduate student. In the beginning also postgraduate students Mikko Alho and Ilkka Saastamoinen made a small contribution to the project. The whole group of Prof. Nurmi currently consists of two post-docs, 10 researchers as postgraduate students and 10 students as research assistants.

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1.3 Funding

Table 1. Funding of the project in 1000 EUR in 2003-2006. Internal funding consists of manpower costs and operational expenditures provided by the organisation. The funding provided by the Academy of Finland and other external sources is also shown in the table.

Partner	Funding organisation	2003	2004	2005	2006	**Total**
TUT	TUT	7	14	14	15	**50**
	Academy		34	46	40	**120**
Total		**7**	**48**	**60**	**55**	**170**

2 Research Work

2.1 Objectives and Work Plan

Efficient platform-based design requires new methodologies to (1) model functional IPs and the communication platform itself, to (2) systematically proceed from an initial system specification to an architecture model composed of a platform model and a set of functional IP models, to (3) map the architecture model to actual concrete IP components in an optimal manner, and to (4) reliably verify, in a number of phases, both functional and timing correctness of the resulting system configuration. The purpose of the CONSTRAIN project was to address these crucial issues. We planned to work on all these areas simultaneously throughout the three-year period 2004-2006 of the project together with University of Turku.

It has to be noticed that the Academy funding is less than 17% of the applied funding which implied some constraints on the project focus. Thus, the main emphasis has been on the communication platform part, especially the XGFT Network-on-Chip.

2.2 Final Report: Common Themes and Collaboration

Collaboration with University of Turku was carried out on unofficial basis since their part was not funded at all by the Academy. The collaboration also produced many joint publications where the credit was given to other projects with more balanced funding basis for cooperation. This includes one Kluwer book on Interconnect-centric design, which also falls into the scope of this project. This project contributed one of the book chapters [2].

2.3 Final Report: Institute of Digital and Computer Systems

A review of arbitration and routing schemes for on-chip communication networks was done and published as a book chapter [2]. The operation of arbitration and routing algorithms has a significant effect on the performance of the packet switched networks. Switch arbiters, which are responsible for scheduling the internal resources of the switches for packet transfers from input ports to output ports, determine the throughput of the switch nodes. Their operation can be modeled with a bipartite graph matching problem where each maximum matching corresponds to a valid schedule with maximum number of simultaneous transfers. Arbitration algorithms can be classified to maximum size matching (MSM) and maximum weight matching algorithms (MWM).

In the book chapter the arbitration was concerned from both theoretic and practical point of view. The arbitration was at first modeled as a maximum matching problem before the different arbitration algorithms were presented. Because current maximum weight matching algorithms have still quite complex and slow hardware implementations, the focus was on maximal size matching algorithms like iSLIP, iDRRM, and WWFA which have smaller and simpler hardware implementations.

Different routing schemes were reviewed after arbitration schemes. Routing algorithms are responsible for controlling the routing of the packets to their desired destinations. The network topology, which can be either regular or irregular, affects the complexity of routing and restricts the set of usable algorithms. Because the operation of the routing algorithms varies along with the network topology, multiple different topologies were also presented briefly. Basically, the routing algorithms are either adaptive or non-adaptive depending on whether they are able to take into consideration the prevailing traffic conditions in the networks when making decisions of the routing paths.

Non-adaptive deterministic routing is usually simpler to implement than adaptive routing which requires distributed decision-making processes at the switch nodes along the routing paths. However, adaptive routing produces typically better performance and for networks with regular topology it has realizable implementations which are not necessarily much more complex than those of non-adaptive routing algorithms.

In a case study at the end of the chapter the earlier presented arbitration and routing schemes were applied to practice in the modified extended generalized fat tree (XGFT) interconnection network. A new adaptive TBWP routing algorithm was introduced and its performance was compared to the performance of adaptive Turnaround routing algorithm. Presented simulation results, depicted in Fig. 1, show that the TBWP routing algorithm can utilize more efficiently all of the available free resources of the network than the Turnaround routing algorithm with slightly increased circuit area, which demonstrates how the operation of the routing algorithm affects the system performance and costs.

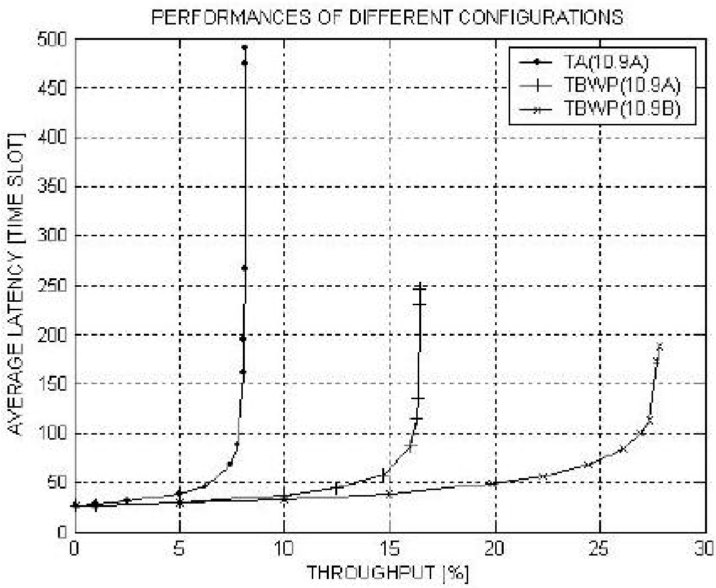

Fig. 1.The performance of different network configurations. TBWP configurations proved to be better than non-adaptive Turnaround algorithm.

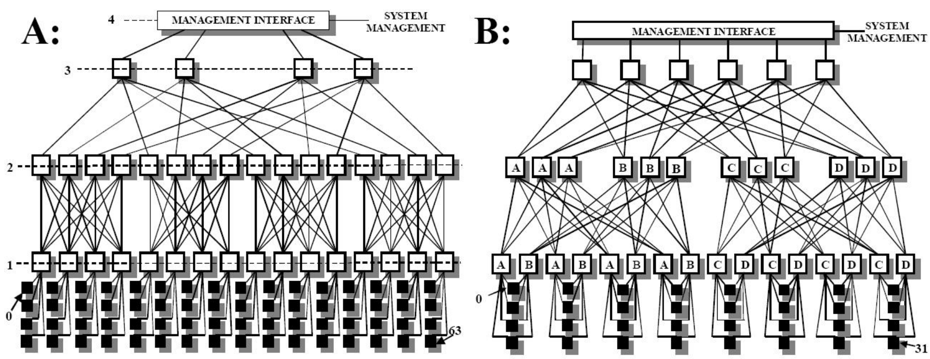

Fig. 2. XGFT(3,4,4,4,4,1,1) (A) and XGFT(3,4,4,4,3,2,1) (B).

The XGFT topology can be defined as XGFT(h, m_1, m_2, ..., m_h, w_1, w_2,..., w_h) tuple where h is the number of switch stages, parameter m_i ($1 \leq i \leq h$) is the number of child nodes of the witch nodes in stage i , and parameter w_i is the number of their parent nodes. Switches in stage one, which is the lowest stage, are connected to processor leaf nodes. Because the degree of switches on different stages of the XGFTs can vary, the XGFTs are more scalable for different system sizes and performance requirements than Fat Trees. This is illustrated in Fig. 2A and 2B where large white squares are switches and small black squares are processor nodes. The stages are numbered in descending order starting from the top of the XGFT, and the leaf nodes are numbered in ascending order starting from the leftmost leaf node. For example, XGFT(3,4,4,4,4,1,1) has more routing resources in its four sub-XGFT(2,4,4,4,1)s than XGFT(3,4,4,4,3,2,1) in its four sub-XGFT(2,4,4,3,2)s. Therefore, it is able to achieve higher throughputs with local cluster traffic. Fig. 1A and 1B depict also how management interfaces, which are actually also switch nodes, could be integrated into different XGFTs.

In the other publications, the XGFT interconnection network is studied further. In [3], two adaptive routing algorithms in this network topology are evaluated and implemented to achieve the physical characteristics of the communication network. Paper [1] is an invited extended journal article based on the previous conference paper. The simulation results in these papers show that both the Turn Back When Possible (TBWP) and Turn Back (TB) routing algorithms produce higher throughputs as the traffic becomes more local.

In [4] the properties of XGFT communications as reusable interconnect IP blocks are discussed. It also introduces a layout scheme for XGFT implementations, shown in Fig. 3. The Flat Switch, which is the darker rectangle within the routing channel, is connected to the switches of the next upper switch layer which is within the XGFT IIP in the middle of the Backbone circuit layout. Flat Switches can be used for reducing the length of the links between the leaf nodes and the lowest switch layer of the XGFT.

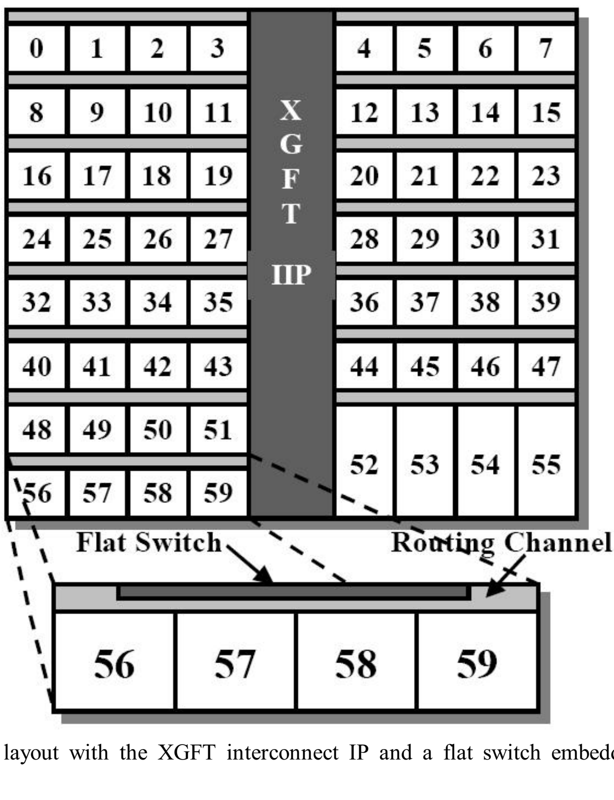

Fig. 3. Backbone layout with the XGFT interconnect IP and a flat switch embedded into a routing channel.

In paper [5] fault tolerance aspects have been introduced to this communication network. The fault tolerance and adaptability are increasingly important in future nanoscale System-on-Chip implementations, where the fault and error probabilities are increasing. This will also have major effect on the industries utilizing semiconductors, and will require a major paradigm shift in the electronics design. Paper [6] further describes the fault-tolerant XGFT and its use for Multi-Processor System-on-Chip (MPSOC) circuits. Because the degree of switches on different stages of the XGFTs can vary, the XGFTs are more scalable for different system sizes and performance requirements than Fat Trees. This is illustrated in Fig. 4A and 4B where large white squares are switches and small black squares are processor nodes. The stages are numbered in descending order starting from the top of the XGFT, and the leaf nodes are numbered in ascending order starting from the leftmost leaf node. For example, XGFT(3,4,4,4,4,1,1) has more routing resources in its four sub-XGFT(2,4,4,4,1)s than XGFT(3,4,4,4,3,2,1) in its four sub-XGFT(2,4,4,3,2)s. Therefore, it is able to achieve higher throughputs with local cluster traffic. Fig. 1A and 1B depict also how management interfaces, which are actually also switch nodes, could be integrated into different XGFTs. XGFTs have a lot of redundant routing resources which are switches and bi-directional transmission links, which can be utilized in improving the fault-tolerance of the XGFTs. Fig. 4B illustrates how the fault tolerance of the system could be improved by using two network interfaces at each of the leaf nodes. Switches in stages one and two have been labeled with letters A, B, C, and D in order to show which sub-XFT of height two they belong to. In this interconnection scheme all of the interfaces have different addresses and it would be possible to transfer packets between any pair of two leaf nodes although e.g. all of the switches and links of sub-XGFTs A and C would be defected. Furthermore, if any of the switches of stages three or two of the XGFT(3,4,4,4,4,1,1)would be defected, there would still be completely functioning switches and links in the network for communication between any pair of processor leaf nodes. This interconnection scheme also doubles the peak bandwidth usable by every processor although there would be two processors in every leaf node.

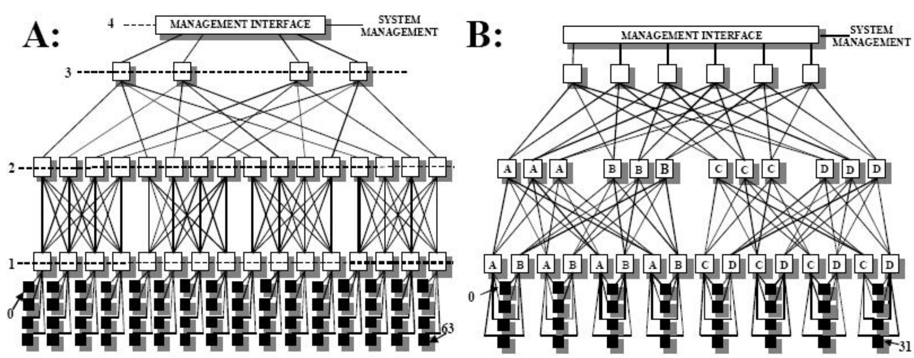

Fig 4. XGFT(3,4,4,4,4,1,1) (A) and XGFT(3,4,4,4,3,2,1) (B).

In paper [7] the developed Fault Detection And Repair (FDAR) system is applied for 2-D Mesh networks and for Full Mesh that was developed to support more processing nodes with the same number of switches as in a conventional 2-D Mesh. This is illustrated in Fig. 5. The paper also presents implementation characteristics of the FDAR system in Mesh type of networks. Synthesis results in a 130 nm technology are shown in Table 2. Generally the FDAR increases the block areas by only about 12% (10-15%). The Full Mesh configuration saves resources. For example, with full 6×6-Mesh it is possible to implement 67% larger system than with conventional mesh. On the other hand, the conventional Mesh of the system of 60 processors would be 67% larger than the Full Mesh of the system of the same size.

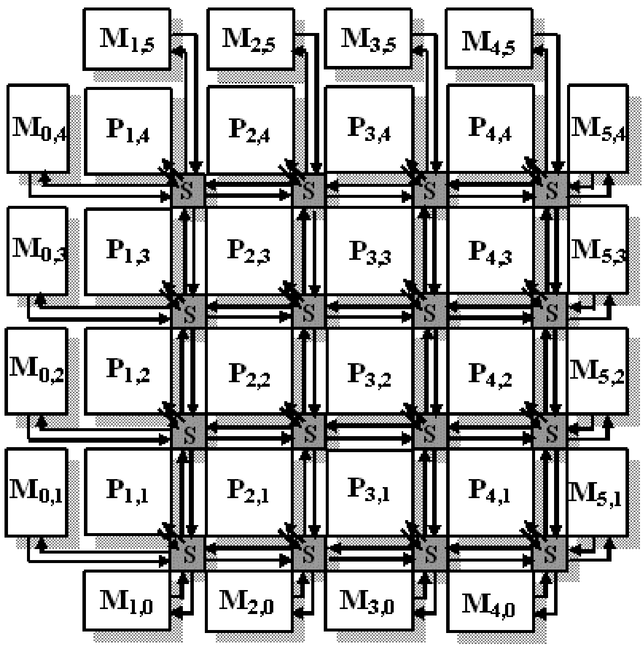

Fig. 5. In full 2-D mesh configuration edge and corner switches can be used for connecting more processors to the network. The number of processors can be N × (N + 4).

Table 2. Synthesis results with and without FDAR.

Block	Without FDAR & FTDOR	With FDAR & FTDOR	Size(full)/ Size(conv.)
5×5-switch	0.233 mm2	0.261 mm2	-
2×2-mesh	0.932 mm2	1.044 mm2	12 / 4 = 3
4×4-mesh	3.728 mm2	4.176 mm2	32 / 16 = 2
6×6-mesh	8.388 mm2	9.396 mm2	60 / 36 = 1.67
8×8-mesh	14.912 mm2	16.704 mm2	96 / 64 = 1.5

Paper [8] summarizes the fault tolerant reconfigurable XGFT network implementation. The network uses switches with distributed modular architecture, as shown in Fig. 6. Every input port (IP) and output port (OP) forms a unidirectional port. The figure also illustrates connections towards child nodes (C) and parent nodes (P). Two unidirectional ports, e.g., $P_{UR}[0]$ and $P_{DR}[0]$, form a bi-directional port.

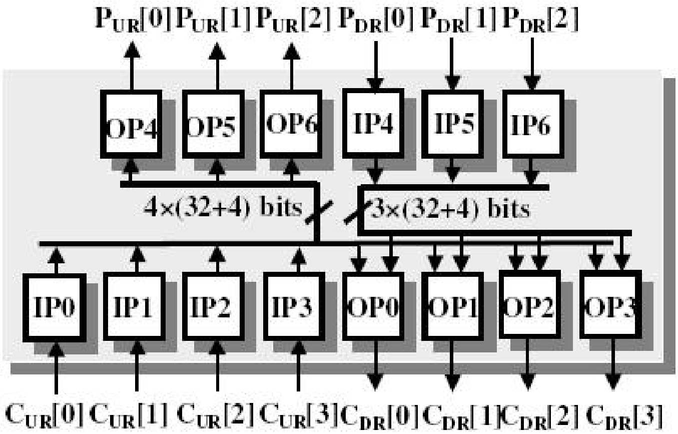

Fig. 6. The structure of a 3x4-switch.

The FDAR system works in two modes: diagnostic mode and normal operation mode. FDAR uses parity checks and timeout counters to detect bit errors and non-functional connections. The switch nodes include logic for locking ports, as shown in Fig. 7. The figure depicts a node for Mesh networks as can be seen from the port naming. The routing, arbitration and switching are distributed to port blocks, there are no centralized blocks in the switches for performing these functions.

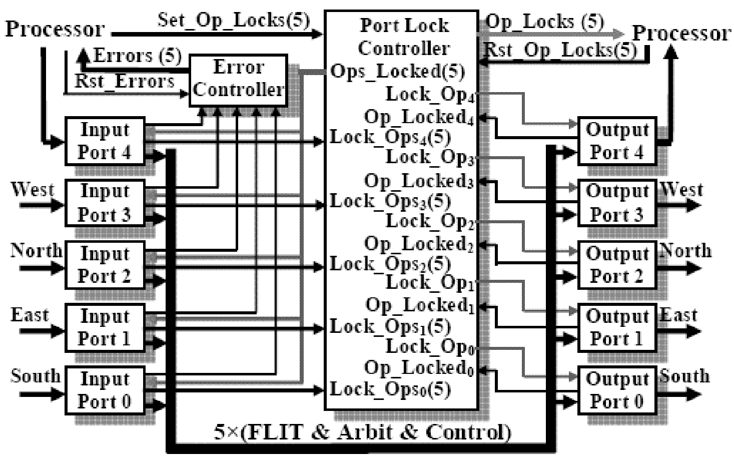

Fig. 7. Distributed switch architecture for Mesh networks.

The Dr.Tech. Thesis of Heikki Kariniemi [9] is a monograph but is based on the eight publications. The thesis was pre-reviewed by Prof. Axel Jantsch from KTH, Stockholm, and Prof. Jouni Isoaho from University of Turku, Finland. Prof. Isoaho and Prof. Johan Lilius from Åbo Akademi University, Turku, Finland were the opponents in the thesis defense in September 2006 at TUT.

3 International Aspects

The research group completed the successful SoC-Mobinet EU project and SoC-SME Nordic/Baltic project (with participant from all eight Nordic and Baltic countries) during 2004. Another European project with co-funding from GJU (Galileo Joint Undertaking) called GREAT (Galileo REceiver for mAss markeT) is underway (March 2006 – March 2008). In 2007, several applications for EU funding in the FP7 are planned.

The group is also otherwise actively cooperating in Europe and worldwide. E.g. KTH (Sweden), Infineon Technologies AG (Austria), Bologna University (Italy), Catena Radio Design BV (The Netherlands), Berkeley Wireless Research Center (USA), and Carinthia Tech Institute (Austria) are key partners. The forms of cooperation include projects, networks, practical research and education cooperation, researcher exchange and shorter visits, and joint organization of events.

4 Publications and Academic Degrees

Table 3. Publications and academic degrees produced in the project. Numbers of different types of publications are given along with the reference numbers. List of refereed journal articles are given in Section 6.1, refereed conference papers in Section 6.2, monographs in Section 6.3 and theses in Section 6.4.

Partner	Type of publication	2003	2004	2005	2006	**Total**	Publication numbers
TUT	Ref. journal art.	-	1	-	-	**1**	1
	Ref. conf. papers	-	3	2	2	**7**	2-8
	Monographs	-	-	-	-	**0**	
	Doctoral dissert.	-	-	-	1	**1**	9
	Licentiate degrees	-	-	-	-	**0**	
	Master degrees	-	-	-	-	**0**	

5 Other Activities

The group has organized solely four international conferences in Tampere, Finland during the project: International Symposium on System-on-Chip in November 16-18 2004 (**SoC 2004**), November 15-17 2005 (**SoC 2005**), November 14-16 2006 (**SoC 2006**), and International Conference on Field-Programmable Logic and Applications (**FPL 2005**) in August 24-26 2005. In addition to being the general chair of these events, Prof. Jari Nurmi was also technical co-chair of European Workshop on Microelectronics (**EWME 2005**) in Stockholm, Sweden in June 2005 and **NORCHIP 2005** conference in Oulu, Finland in November 2005.

Prof. Jari Nurmi was invited to give talks on the System-on-Chip design challenges and Networks-on-Chip in the Swedish System-on-Chip Conference 2005 [13], International Symposium on System-on-Chip 2005 [14], and Multi-Processor System-on-Chip Forum 2006 [15].

The groups from Tampere University of Technology and University of Turku are organizing annually a joint seminar to the industry. The seminars taking place during the project were held in Turku 22.4.2004 (Complain project final seminar), in Tampere in 7.3.2005 (AVEC project annual seminar), and in Tampere again 13.2.2006 (AVEC).

Prof. Nurmi also presented the project in TULE programme final seminar [16].

6 Publications

6.1 Refereed Journal Articles

[1] Heikki Kariniemi and Jari Nurmi, "Performance Evaluation and Implementation of Two Adaptive Routing Algorithms for XGFT Networks," in *Computing and Informatics*, vol. 23, no. 5-6, 2004, pp. 415-435, ISSN 1335-9150, Slovak Academic Press Ltd., Bratislava, Slovakia.

6.2 Refereed Conference Papers

[2] Heikki Kariniemi and Jari Nurmi, "Arbitration and Routing Schemes for On-Chip Packet Networks," in J. Nurmi, H. Tenhunen, J. Isoaho, A. Jantsch, (Eds.), ISBN 1-4020-7835-8, *Interconnect-Centric Design for Advanced SoC and NoC*, Kluwer Academic Publishers, 2004, pp. 253-282.

[3] Heikki Kariniemi and Jari Nurmi, "Performance Evaluation and Implementation of Two Adaptive Routing Algorithms for XGFT Networks," in *Proc. The 7th IEEE International Workshop on Design and Diagnostics of Electronic Circuits and Systems DDECS'04*, Tatranska Lomnica, Slovakia, April 18-21, 2004.

[4] Heikki Kariniemi and Jari Nurmi, "Reusable XGFT Interconnect IP for Network-On-Chip Implementations," in *Proc. International Symposium on System-on-Chip SoC2004*, Tampere, Finland, November 16-18, 2004, pp. 95-102.

[5] Heikki Kariniemi and Jari Nurmi, "Versatile Modular Switch Architecture for Improving the QOS of the XGFT Network-on-Chip," in *Proc. The 8th IEEE Workshop on Design and Diagnostics of Electronic Circuits and Systems DDECS 2005*, Sopron, Hungary, April 13-16, 2005, pp. 105-112.

[6] Heikki Kariniemi and Jari Nurmi, "Fault-Tolerant XGFT Network-on-Chip for Multi-Processor System-on-Chip Circuits," in *Proc. International Conference on Field Programmable Logic and Applications FPL 2005*, Tampere, Finland, August 24-26, 2005, pp. 203-210.

[7] Heikki Kariniemi and Jari Nurmi, "Fault-Tolerant 2-D Mesh Network-on-Chip for Multiprocessor Systems-on-Chip," in *Proc. IEEE Workshop on Design and Diagnostics of Electronic Circuits and Systems DDECS 2006*, Prague, Czech Republic, April 18-21, 2006, pp. 186-190.

[8] Heikki Kariniemi and Jari Nurmi, "On-line Reconfigurable XGFT Network-on-Chip Designed for Improving the Fault Tolerance and Manufacturability of the MPSOC Chips, in *Proc. International Conference on Field Programmable Logic and Applications FPL 2006*, Madrid, Spain, August 28-30.

6.3 Monographs

none

6.4 Doctoral, Licentiate, and Master Theses

[9] Heikki Kariniemi, *On-Line Reconfigurable Extended Generalized Fat Tree Network-on-Chip for Multiprocessor System-on-Chip Circuits*, **DrTech Thesis**, Tampere University of Technology, September 2006, ISBN 952-15-1651-8, ISSN 1459-2045. TUT Publication 614.

7 Other References

[10] Jari Nurmi, Hannu Tenhunen, Jouni Isoaho, and Axel Jantsch (Eds.), *Interconnect-Centric Design for Advanced SoC and NoC*, Kluwer Academic Publishers, 2004, ISBN 1-4020-7835-8.

[11] Heikki Kariniemi and Jari Nurmi, "Fault-Diagnosis-and-Repair System for Improving the Fault-Tolerance and Manufacturability of MPSoCs," abstract in the *Workshop on Future Interconnects and Networks on Chip at DATE 2006*, Munich, Germany, March 10, 2006.

[12] Heikki Kariniemi and Jari Nurmi, "Versatile XGFT Network-on-Chip with Improved Fault-Tolerance and Manufacturability of MPSoCs," abstract in the *Workshop on Future Interconnects and Networks on Chip at DATE 2006*, Munich, Germany, March 10, 2006.

[13] Jari Nurmi, "Challenges of System-on-Chip in Nanoscale Technologies," invited presentation in *Swedish System-on-Chip Conference SSoCC'05*, Tammsvik, Sweden, April 19, 2005.

[14] Jari Nurmi, "Network-on-Chip: A New Paradigm for System-on-Chip Design," invited paper in *Proc. International Symposium on System-on-Chip SoC 2005*, Tampere, Finland, November 15-17, 2005, pp. 2-6.

[15] Jari Nurmi, "Challenges of MPSOC Communication, Computation and Design Flow," invited in-depth presentation in *Multi-Processor System on Chip Forum (MPSOC 2006)*, Estes Park, Colorado, USA, August 14-18, 2006.

[16] Jari Nurmi, "Constraint-Driven Platform-Based System-on-Chip Design," presentation in *Academy of Finland TULE Programme Final Seminar*, Helsinki, Finland, December 12, 2006.

DYNAMIC PARALLEL RADIO STRUCTURES FOR CELL ARRAY PLATFORMS (ARRAYRADIO)

Professor Jouni Isoaho, University of Turku, Communication Systems

Abstract

The essential target of the project is to develop radio structures and algorithms that are easily mappable to parallel architectures, especially cell array platforms, and support dynamic reconfiguration and error-tolerance. Easy and efficient mappability is achieved by building the system from parameterisable homogenous seed cells with highly concurrent operations. In this project, the main effort is on developing autonomous concurrent radio solutions for array platforms. The diversity techniques and multiple-input multiple-output (MIMO) antenna system approaches are used as basic radio technologies. Radio algorithms/architectures are formed to support system and component level modularity for efficient design flow, reconfigurability and architecture matching. The techniques for dynamic reconfiguration of radio systems are developed to optimise system performance and power consumption. An agent-based approach is used to ensure that the system works in error-free manner, although the basic building blocks can be defective due to static and dynamic errors or failures. This means that error correction and fault-tolerance aspects are considered in all three levels: algorithms, architectures and technology platforms.

1 Partners and Funding

1.1 Communication Systems, University of Turku

1.1.1 Background and Mission

The laboratory is responsible for teaching and research of communication systems. The target is to develop key enabling technology and competence needed for designing and implementing broadband digital communication and computation systems today and in future. This includes integration of wireless and wired communication infrastructures with dynamic system implementation techniques and platforms. System design methodologies cover both functional and physical design and modelling issues. To achieve goal given the development of research and teaching activities are strongly integrated. Also, laboratory has taken strong role in co-operation and networking within its key areas. The laboratory co-operates actively with Tampere University of Technology, Finland, and the Royal Institute of Technology, Sweden.

1.1.2 Research

In research activities laboratory has focused in three main issues:

- Basic technologies
    - Radio systems and algorithms, mobile technology, coding technology, data security
    - Speech and interface technologies, geographical information systems
    - Intelligent agents, self/context-aware systems
- Human and society interactivity
    - Human driven technology development
    - Technology for promoting human activity in society processes
- Implementation technologies
    - Software defined mobile terminals
    - Algorithms and systems for nano-scale technologies
    - Distributed/networked system implementations

In addition to this new approach to nano and software defined radio systems, there is currently two other important group of activity areas with several projects. In communication technology the other focus is currently on IP datacasting for mobile receivers. The Dtv group of communication systems laboratory (http://www.dtvgroup.fi) has strong international impact via standardization, pan-European consortiums (Eureka/Celtic, COST, eMobility, NEM), and close contacts with industry partners. Dtv group's R&D covers whole end-to-end chain of mobile datacasting systems including all protocol layers. A transmission and service distribution system utilizing converged broadcast/cellular networks is implemented in practice to provide a testing platform for new services. The third high priority activity area is speed and language technology where the laboratory is co-ordinating large national project in speech technology, and has very active role in creation of a new technology cluster in the field of multi-culture communication and understanding.

1.2 Funding

Table 1. Funding of the project in 1000 EUR in 2004-2006. Internal funding consists of manpower costs and operational expenditures provided by the organisation. The funding provided by the Academy of Finland and other external sources is also shown in the table.

Partner	Funding organisation	2004	2005	2006	**Total**
	Academy	34	46	40	**120**
	Industry and Tekes	38	40	38	**116**
Total		**72**	**86**	**78**	**236**

2 Research Work

2.1 Objectives and Work Plan

In the project there were three major problems to be solved: (i) how to make systems easily implementable with highly parallal platforms, (ii) how to make radio systems autonomous and reconfigurable, and (iii) how to build robust, error-free and highly scalable systems, when basic building blocks can be defective due to static and dynamic errors or failures.

2.2 Final Report: Common Themes and Collaboration

Research themes can be split to areas: (1) radio approach and algorithms, (2) parallel implementation platforms and (3) agent technology. The key innovations we have been working on in this project are:

- **Self-design**. Extending design methodologies from actual design phase to self-design.
- **Unlimited scalability**. Solving yield and design methodology limitations to exploit highly parallel and highly homogenous platforms. This needs work with algorithms, system concepts and architectures (towards homogenous processing units).
- **Design layers and abstractions.** A new meta-design layer to provide system level intelligence to ensure dynamic use of resources and reliable implementations in non-robust technology basis.

Here those innovations are processed in the context of software defined radio application. At first, promising candidates for future radio and application algorithms and architectures are evaluated providing required performance and flexibility needs. These evaluation results are used to specify demands for actual implementation platforms. To platform implementations we approach by integrating three different platform approaches: (1) a single or multiprocessor general core processors providing highest flexibility and lowest performance, (2) parallel array processors with quite fixed structures having very high performance with very limited online flexibility in programmability and architectural mapping, and (3) as a compromise Transport-Triggered Architecture to integrate heterogeneous type of modules and implementation topologies in quite efficient manner still with some limitations in flexibility. Implementation trade-offs also with fixed, reconfigurable and programmable solutions. There the key study there will be the definition of fixed and non-fixed structures and operations to provide optimal performance and flexibility trade-offs.

In addition to capacity increase, the new technologies introduce also completely new problems. How to build robust, error-free and highly scalable systems, when basic building blocks can be defective due to static and dynamic errors or failures. This means that our approach needs to consider error correction and fault-tolerance aspects in all three levels: algorithms, architectures and technology platforms. Management for reconfiguration and fault-tolerance is based on the agent technology. An agent function, which is added to an application function, composes a component abstraction that interacts with environment through sensors and actuators. The overall system is composed by a set of co-operative or competitive agents. An agent hierarchy used is based on four different levels: application, platform, cluster and cell. The application agent is used to recognise application needs for system reconfiguration, e.g. due to change of functionality, fault-tolerance or performance enhancement. The platform agent forms interface between application and platform. The cluster agent performs reconfiguration if necessary based on request either from cell or application level. The cell agent takes care of routing and cell diagnostics. A fault-tolerant agent based radio structure is presented in Figure 1. There the diversity techniques are used in parallel radio structure with dynamically adjusted amount of parallelism in order to guarantee best possible performance under rapidly changing mobile channel and unreliable hardware. The demonstration platform hierarchy is presented in Figure 2. Overall system demonstrators will be finalised during 2007.

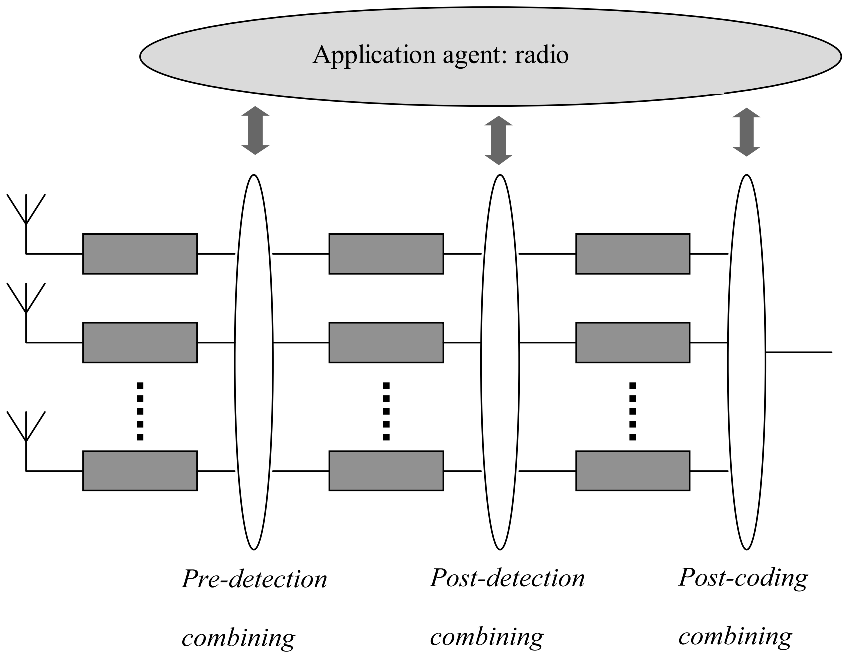

Fig. 1. Agent based radio structure.

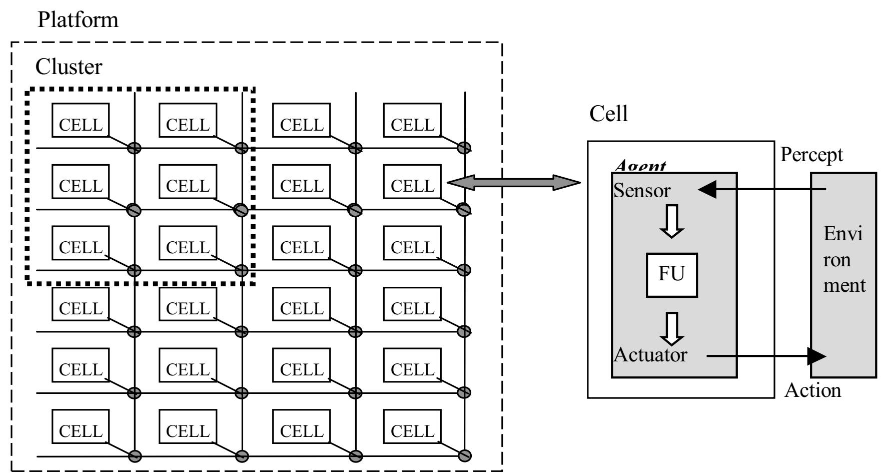

Fig. 2. Platform hierarchy.

3 International Aspects

We submitted project proposal for FET/STREP in 2005. Topic was Integrated Autonomous Self-Aware Nanoelectronics (INSANE). The initiative for this proposal was based on work in done in this ArrayRadio project. The developed radio approach was target to be key application in INSANE project. Partners were Royal Institute of Technology (KTH), Technische Universiteit Delft (TUDelft), Institut national polytechnique de Grenoble (INPG), Ecole Polytechnique Federale de Lausanne (EPFL), and University of Turku. Unfortunately, although we succeeded to the second application round, we didn't receive any funding for the project from EU. We are currently planning to resubmit the proposal to new EU frame programme.

4 Publications and Academic Degrees

Table 2. Publications and academic degrees produced in the project. Numbers of different types of publications are given along with the reference numbers. List of refereed journal articles are given in Section 6.1, refereed conference papers in Section 6.2, monographs in Section 6.3 and theses in Section 6.4.

Partner	Type of publication	2004	2005	2006	**Total**	Publication numbers
TUT	Ref. journal art.	-	-	1	**1**	1
	Ref. conf. papers	-	6	1	**12**	2 - 8
	Monographs	1	-	-	**1**	9
	Doctoral dissert.	1	-	-	**1**	10
	Master degrees	1	1	1	**3**	11 – 13

5 Other Activities

This project results has been presented in annual research seminars for Finnish Industry organised jointly with Professor Jari Nurmi, Tampere University of Technology. Project results are used to push up new research and educational direction in nanosystems design. The concept developed during this project was also presented by prof. Isoaho as an invited presentation at 6th Workshop on Microelectronics Education (EWME) in Stockholm. The topic of the presentation was “Towards Integrated Autonomous Self-Aware Nanoelectronics Education”.

6 Publications

This project was the start-up of a new era in software defined radio development and nanosystems design. During the project the key research group was established and therefore the most meaningful scientific contributions relating to project results will be published during 2007-8.

6.1 Refereed Journal Articles

[1] Muhammad Imran Anwar, Seppo Virtanen and Jouni Isoaho. A Software Defined Approach for Common Baseband Processing. Submitted to Journal of System Architecture, Elsevier, Aug. 2006.

6.2 Refereed Conference Papers

[2] Jani Paakkulainen, Seppo Virtanen and Jouni Isoaho. Tuning a Protocol Processor Architecture Towards DSP Operations. In *5th International Workshop on Embedded Computer Systems (SAMOS V)*, Jul 2005.

[3] Petri Isomäki and Nastooh Avessta. Rapid Refinable Software Defined Radio Design. In *2nd International Symposium on Wireless Communication Systems, 2005.* , Sep 2005.

Appaya Devaraj Swaminathan and Nastooh Avessta. Array Processors for Viterbi Decoder. In *2nd International Symposium on Wireless Communication Systems 2005 (ISWCS2005)*, 2005.

[4] Jouni Isoaho, Pekka Rantala, Tero Nurmi and Hannu Tenhunen. New Course on Computational Platforms towards Nano-Scale Systems. In *Proceedings of the 23rd Norchip Conference (NORCHIP-05)*, Aug 2005.

[5] Seppo Virtanen, Dragos Truscan, Jani Paakkulainen, Jouni Isoaho and Johan Lilius. Highly Automated FPGA Synthesis of Application-Specific Protocol Processors. In *Proceedings of the*

15th International Conference on Field Programmable Logic and Applications (FPL 2005), Aug 2005.

[6] Petri Isomäki and Nastooh Avessta. Rapid Refinable SoC SDR Design. In *2005 International Symposium on System-on-Chip*, Nov 2005.

[7] Muhammad Imran Anwar and Seppo Virtanen. Mapping the DVB Physical Layer onto SDR-enabled Protocol Processor Hardware. In *Proceedings of the 23rd IEEE Norchip Conference*, Nov 2005.

[8] Teijo Lehtonen, Pekka Rantala, Petri Isomäki, Juha Plosila and Jouni Isoaho. An Approach for Analysing and Improving Fault Tolerance in Radio Architectures. In *Proceedings of IEEE International Symposium on Circuits and Systems ISCAS 2006*, May 2006.

6.3 Monographs

[9] Jari Nurmi, Hannu Tenhunen, Jouni Isoaho and Axel Jantsch. Interconnect-Centric Design for Advanced SoC and NoC, 2004.

6.4 Doctoral, Licentiate, and Master Theses

[10] Seppo Virtanen. A Framework for Rapid Design and Evaluation of Protocol Processors. PhD thesis, Sep 2004.

[11] Jani Paakkulainen. Esisuodatus digitaalisella rinnakkaislaskentaverkolla. Master thesis. Department of Information Technology. University of Turku. 2004.

[12] Muhammed Imran Anwar. Implementation of Software Defined Radio on TACO Processor Architecture using DVB.-T and DVB-H Technologies. Master thesis. Department of Information Technology. University of Turku. 2005.

[13] Appaya Devaraj Swaminathan. Mapping Uniform Reccurrence Equations to Systolic Arrays. Master thesis. Department of Information Technology. University of Turku. 2006.

7 Other References

[14] Tapani Ahonen, Seppo Virtanen, Juha Kylliäinen, Dragos Truscan, David Sigüenza-Tortosa, Jani Paakkulainen, Tapio Ristimäki, Tuukka Kasanko, Tero Nurmi, Hannu Isännäinen, Ilkka Saastamoinen, Johan Lilius, Jari Nurmi and Jouni Isoaho. A Brunch from the Coffee Table - Case Study in NoC Platform Design. In Interconnect-centric Design for Advanced SoC and NoC. J. Nurmi, H. Tenhunen, J. Isoaho and A. Jantsch, editors. , chapter 16. Kluwer Academic Publishers, Apr 2004.

[15] Petri Isomäki, Pekka Rantala, Devaraj Swaminathan, Nastooh Avessta, Juha Plosila and Jouni Isoaho. Radiopiireihin rinnakkaisuutta. *Prosessori*, (13):52-54, Nov 2004.

[16] Petri Isomäki and Nastooh Avessta. An Overview of Software Defined Radio Technologies. Technical Report 652, TUCS, Dec 2004.

HeWiT – High Efficiency Wideband Transmitters

Timo Rahkonen[1] , Saska Lindfors [2].

Abstract

The project aimed in gathering experience and new circuit-level and signal processing solutions for the design of polar RF transmitter architectures, that have potential to a very high power efficiency. The polar transmitter consists of a switched RF power amplifier that amplifies the phase information of the carrier, a modulated supply voltage to add the amplitude information, and digital signal processing to separate the phase and amplitude components and add time-aligning and predistortion operations when needed. Such a system was analysed by extensive behavioural simulations, where the required specifications of each part were searched. Then, a test setup was built, consisting of a 0.5W, 1 GHz class E power amplifier, a 1W supply modulator and a data sequencer built on an FPGA card, all made of commercial components. The system was tested, and the main nonidealities were recognised. To correct those, various signal processing algorithms were developed, resulting at best in 20 dB improvement in adjacent channel leakage. An alternative implementation of the supply modulator was designed which relies on digital signal processing rather than analog feedback. Finally, a digital implementation of the baseband signal processing was designed.

1 Partners and Funding

1.1 Electronics Laboratory, University of Oulu (OU)

The research group consists of subproject leader professor Timo Rahkonen, and three students / postgraduate students DI Simo Hietakangas, DI Timo Rautio, and DI Olli-Pekka Jokitalo. The group was partly funded by a parallel TEKES project.

1.2 Circuit Design Laboratory, Technical University of Helsinki (HUT)

The research group consists of subproject leader professor Saska Lindfors, and one postgraduate student DI Mikko Talonen..

1.3 Funding

The project was planned for years 2005-2006, and its budget was 120 000 EUR for Oulu and 120 000 for HUT (ca. 2/3 of the applied funding). The work in Oulu was supported by a TEKES project DISTO05 (funded by National Semiconductor Finland, Elektrobit, Esju, and Aplac) that was partly in the same area. This allowed to have a sufficient staff to build a complete transmitter, with one student working on the RF PA, one on DSP, and one on the supply modulator. Although the TULE project was not originally planned

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[2] Circuit Design Laboratory, Technical University of Helsinki, PO.Box 111, FIN-22222 Espoo

to co-exist with this TEKES project, the contribution of the latter was essential and is hence shown here. However, only ca. 40 % of the TEKES project shown was related to this TULE project.

Table 1. Funding of the project in 1000 EUR in 2003-2006. Internal funding consists of manpower costs and operational expenditures provided by the organisation. The funding provided by the Academy of Finland and other external sources is also shown in the table.

Partner	Funding organisation	2003	2004	2005	2006	**Total**
OU	Academy	-	-	60	60	**120**
	TEKES	-	-	60	35	**95**
	Industry	-	-	0	24	**24**
HUT	Academy	-	-	60	60	**120**
Total		**-**	**-**	**180**	**159**	**339**

2 Research Work

2.1 Objectives and Work Plan

In all linear power amplifiers, the power efficiency drops rapidly with reduced signal level, which results in low overall efficiency with modern efficient modulation formats. The overcome this efficiency bottleneck, the main objective of this project was to develop circuit technology for wideband RF polar transmitters. A polar transmitter employs a switching RF power amplifier with close to 100% power efficiency. The input to a switching amplifier has a constant envelope (and hence a broad spectrum), but in the polar transmitter it has a modulated supply voltage to allow also the amplitude modulation of the signal. Thus, the overall hardware of the transmitter consists of a nonlinear switching power amplifier, a broadband modulated power supply, and digital signal separation and predistortion block, as shown in Figure 1.

The main expected contributions of the project were:

1) recognise, analyse, model, and understand all the important nonlinear effects in a polar transmitter,
2) find circuit level and signal processing solutions to minimise these effects, and
3) verify these solutions in practice.

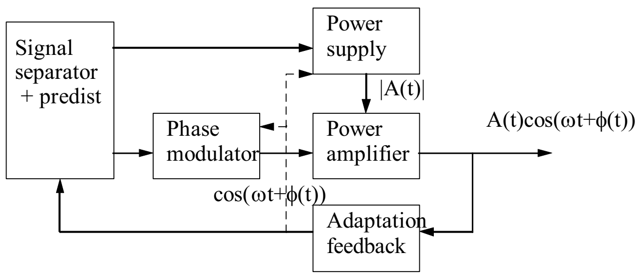

Fig. 1. Block diagram of a polar transmitter.

To achieve these, a polar modulator architecture was analysed, and a prototype was built and tested. Also developing characterisation environment and digital signal processing blocks for a polar transmitter were planned. Originally, the research work was divided into following tasks:

HUT1a: Implementation of a system simulation model of a polar transmitter. This was completed during 1-2Q05 and the results are published in [4].
HUT1b: Implementation of a hardware test bed and system tests.
HUT2a: Development of signal generation.
HUT2b: Development of error detection.
UO1: The RF power amplifier. This was completed during 2005 and is reported in [2,6].
UO2: The modulated power supply. This was completed by summer 2006 and is reported in [1,8].

Besides the tasks listed above, a complete test setup consisting of commercial FPGA, D/A converters and IQ modulator was built in Oulu in the parallel TEKES project. During 2006, it was used to develop and experiment digital error correction schemes for a polar transmitter. These results are reported in [3,7].

2.2 Final Report: Common Themes and Collaboration

The tasks in the project were divided to complement but not seriously overlap with each other. First, a system model of a polar transmitter was built in HUT, and required parameters for a WLAN transmitter were sought out. More detailed description of each task is given in the following sections. Based on the obtained specifications, somewhat reduced specs suitable for a WCDMA signal were taken as a starting point in Oulu, and a class E amplifier and a modulated power supply were designed and tested. Extra samples of the RF PA and the supply modulator were sent to HUT to be characterised in the measurement setup. Due to better funding resources, a complete transmitter was built in Oulu, and the the signal processing methods were studied there using Matlab generated and predistorted data, while digital implementation for a base-band signal processing of a polar modulator was designed in HUT.

2.3 Final Report: Electronics Laboratory, University of Oulu

The first task in Oulu addressed the design of a class E switch-mode RF power amplifier, and especially its use in a polar transmitter. A 1 GHz, 0.5 W prototype was designed and built using a discrete MESFET transistor, and the results are reported in [2],[6], and shortly summarised here. The main findings were: 1) A class E amplifier needs a transistor with low output capacitance, low Ron, and a package with low parasitics, as these very easily ruin the pulse-shaping that class E operation is based on. 2) Modulation bandwidth of a class E amplifier is set by the drain DC biasing network. 3) Main non-idealities of a class E amplifier are the input-output feedthrough that causes both leakage of the broadband input signal, and severe (50-70 degrees) AM-PM distortion at low amplitudes, and AM compression due to saturation of the switch transistor.

The supply voltage modulator needs to have both a large bandwidth and a high power efficiency, and a combination of an asynchronous Buck switch-mode regulator and an assisting broadband video amplifier was chosen. Such a circuit is very slow to simulate, however, and an effective simulation method based on state analysis was developed to explore the design space. This analysis showed that the optimum would be a relatively slow switcher and a very broadband video amplifier, and such a prototype capable for delivering 1W to a 30 ohm load with a bandwidth of several MHz was built using discrete components. The design method and test results are reported in detail in [1],[8], and the most important finding was that a very broadband assisting amplifier is needed to keep the output impedance and hence the ripple voltage of the modulator low enough.

To test the transmitter, a digital signal separator and RF carrier generation was needed. This was implemented by building a four-channel 40 Msamples/s data sequencer on an FPGA with on-board RAM, converting the controls to analog using a self-made D/A board, and upconverting the carrier using a commercial IQ-modulator board. The output signal was recorded using Rohde&Schwarz FSQ signal analyzer, and the input data was generated in Matlab, where various predistortion techniques were experimented to cancel the input-output feed-through and large residual AM-PM. With these corrections applied, the spectral purity was improved by 20 dB. The test environment and some measured results are reported in [3],[7].

2.4 Final Report: Electronic Circuit Design Laboratory, Helsinki University of Technology

Task was to design and implement base band circuitry for wide band polar transmitter. IEEE 802.11a WLAN was chosen to be target system because of its relatively wide bandwidth. It uses also orthogonal frequency division multiplexing (OFDM) modulation that is widely used in modern communications standards.

The first task was to create a system level simulation test bench to define different performance requirements for WLAN polar transmitter. The simulation bench can be used to design appropriate predistortion algorithms for the power amplifier, but this requires a good power amplifier model. In the first phase of system level simulations, a very simple static PA model was used. This work was reported in [4].

In the next phase it was intended to improve the PA model and to design a PA predistortion system. To develop a model, measurement data of an actual PA was needed. A commercial PA was obtained and a proper measurement setup was developed to capture the dynamic behaviour of the polar PA. The key measurement equipment was Agilent 54855a sampling oscilloscope. With that it is possible to capture time domain signal waveforms from each of the three terminals of the polar PA. The results from the time domain measurement setup were compared with traditional measurements that were performed with a vector network analyzer. The results from both measurements were in a good consistency. The results, however, showed that the obtained PA was not suitable for our purposes, which was also later verified by the PA manufacturer. Modelling work was carried out in parallel with measurements with a transistor level PA model with some explicitly embedded memory to emulate thermal effects. A memory polynomial model was tried to capture the dynamic behaviour of the transistor level PA model, but it did not perform satisfactorily. After these experiments it was decided, due to lack of time, to abandon the modelling work and proceed with test bed implementation.

As mentioned previously, a wide band power supply modulator is needed in the polar transmitter. In [9] split-band modulator structure was presented to be one potential structure. The split-band modulator divides the envelope signal into two frequency bands. Both signal paths are amplified separately. High efficiency results from the fact that most of the power of the envelope signal is at the low frequencies and this part can be amplified with a very high efficiency. These two bands are then combined with passive filters. Solution presented in reference [9] is partially incomplete as it does not give any implementation details. Split-band modulator structure was further developed and results are presented in reference [5]. The designed split-band modulator has a nearly flat amplitude response and linear phase response. Furthermore, it achieves nearly perfect isolation in a passive diplex filter.

Digital part of the hardware test bed was implemented with a commercial FPGA board. Envelope signal can be converted to analog domain with on board DAC. Phase signal is fed to separate board with two DACs and IQ-modulator that was designed and implemented as a part of the project.

The required DSP consists of a 64-point IFFT processor, upsampling filter, coordinate transformation block, PA predistortion block, magnitude and phase response and delay equalization filters. Also an interface with PC is required to control different blocks during the measurements. Control software for PC was written and an interface circuit on FPGA was created. The IFFT processor was implemented with a hardware efficient radix-2^2 single delay feedback structure. The upsampling by eight was implemented with three poly phase filters that each upsamples signal by a factor of two. Cartesian I-and Q-signals were transformed to the envelope and to phasor signals with a very hardware efficient structure that included two CORDIC structures. The implementation of the remaining DSP blocks will extend into 2007.

3 International Aspects

The research groups have attended to several international conferences, and have been active in organisation and review work. T. Rahkonen was the technical chair of Norchip 2005 conference (Oulu, Nov 2005) and belonged to technical program committee of InMMIC conference (Aveiro, Portugal, Jan 2006). S. Lindfors was the editor of Norchip 2005 issue of Kluwer Academics journal of analog integrated circuits and signal processing, and arranged a graduate course with international teachers in June 2005. He also maintains good contacts to Aalborg university in Denmark, where his previous PhD student defended his dissertation in February 2006.

Largely based on the experience from this project, T. Rahkonen is part of a circuit simulation related consortium aiming for a FP7 EU project. Also discussions about direct research co-operation have been conducted with Freescale Semiconductors, but with no success.

4 Publications and Academic Degrees

Table 2. Publications and academic degrees produced in the project. Numbers of different types of publications are given along with the reference numbers. List of refereed journal articles are given in Section 6.1, refereed conference papers in Section 6.2, monographs in Section 6.3 and theses in Section 6.4.

Partner	Type of publication	-	-	2005	2006	**Total**	Publication numbers
OU	Ref. journal art.			-	-	**0**	
	Ref. conf. papers			-	3	**3**	[1-3]
	Monographs	-	-	-	-	**0**	
	Doctoral dissert.	-	-	-	-	**0**	
	Licentiate degrees	-	-	-	-	**0**	
	Master degrees	-	-	1	2	**3**	[6-8]
HUT	Ref. journal art.	-	-	-	-	**0**	
	Ref. conf. papers	-	-	1	1	**2**	[4-5]
	Monographs	-	-	-	-	**0**	
	Doctoral dissert.	-	-	-	-	**0**	
	Licentiate degrees	-	-	-	-	**0**	
	Master degrees	-	-	-	-	**0**	

5 Other Activities

S. Lindfors arranged a graduate course in RF circuit design and power amplifier design in Helsinki, June 2005. T. Rahkonen arranged Norchip 2005 conference in Oulu, November 2005.

6 Publications

6.1 Refereed Journal Articles

None.

6.2 Refereed Conference Papers

[1] T. Rahkonen, O-P Jokitalo, Design of a linearly assitend switcher for a supply modulated RE transmitter, Proc Norchip conference, Linköping, 20-21 November, 2006, pp. 1-4.

[2] S. Hietakangas, T. Rautio, T. Rahkonen. 1 GHz class E RF power amplfier for a polar transmitter, Proc Norchip conference, Linköping, 20-21 November, 2006, pp. 5-10.

[3] T. Rautio, S. Hietakangas, T. Rahkonen. Development environment for EER and envelope trasking RF transmitters, Proc Norchip conference, Linköping, 20-21 November, 2006, pp. 151-153.

[4] M. Talonen, S. Lindfors, System requirements for OFDM polar transmitter, European Conference on Circuit Theory and Design ECCTD´05, Cork, Ireland, 29 Aug – 2 Spet 2005, pp.

[5] M. Talonen, S. Lindfors, Split-band supply modulator for OFDM polar transmitter, submitted to ISCAS 2007

6.3 Monographs

None.

6.4 Doctoral, Licentiate, and Master Theses

[6] S. Hietakangas, Käyttöjännitemoduloitavan E-luokan tehovahvistimen suunnittelu. MSc thesis, Department of Electrical and Information Engineering, University of Oulu, 2005

[7] T. Rautio, Polaarilähettimen signaalilähteen ja testiympäristön kehittäminen. MSc thesis, Department of Electrical and Information Engineering, University of Oulu, 2006

[8] O-P Jokitalo. Laajakaistaisen moduloidun hakkurijännitelähteen suunnittelu. MSc thesis, Department of Electrical and Information Engineering, University of Oulu, 2006

7 Other References

[9] F. H. Raab, Split-band modulator for Kahn-technique transmitters, IEEE MTT-S International, June 2004, pp. 887-890

MACMOT: MULTI-ANTENNA CONFIGURATIONS AND TRANSCEIVER STRUCTURES FOR MOBILE TERMINALS

Visa Koivunen[1], Pertti Vainikainen[2], Erkki Salonen[3].

Abstract

The goal of the project was to develop adaptive multiantenna systems for mobile terminals. Multiple antennas are needed because current and future multi-radio mobile terminals may have over 10 radios, each needing an antenna. Moreover, multiantenna systems in both base station and mobile terminals lead to so called Multiple-Input Multiple-Output (MIMO) systems. MIMO systems provide a robust way to significantly improve spectral efficiency (bits/s/Hz) as well as the reliability of a radio link. MIMO the key technology in future beyond 3G and 4G wireless communication systems, where data rates may be up to 1Gbit/s. Multiple antennas in a transceiver tend to occupy plenty of space because typically $\lambda/2$ inter-element spacing is needed. Due to the small size of mobile terminals and other significant implementation limitations, multiple antennas have not been considered to be a feasible option. In an electrically small device, the whole structure contributes to the radiated power making the antenna design complicated.

Availability of new small size antennas, advances in multidimensional channel modeling, availability of MIMO channel measurements, deployment of higher frequencies, development of MIMO system models and diversity techniques have made the use of multiple antenna in a terminal very attractive. New antenna suitable for multiradio systems as well as antenna configurations that occupy less space and yield similar diversity and array gains have been developed. In addition, new smart antenna algorithms and statistical methods for arbitrary antenna configurations have been derived that possess desirable optimality and robustness properties. Low computational complexity and low power consumption are additional design goals for such methods. Availability of extensive propagation channel measurements facilitates creating experimental calculation-based antenna system test-bed where measured and simulated antenna patterns may be compared. In addition, performance tests using 3-D measurement system may be conducted in an anechoic chamber.

1 Partners and Funding

1.1 SMARAD Center of Excellence in Research

The world class educational and research environment in SMARAD center of excellence nominated by the Academy of Finland located at the Department of Electrical and Communications Engineering (ECE), Helsinki University of Technology, encourages students and faculty to participate in research as a group and forming international research networks.
The following two research groups from the SMARAD center of excellence from HUT are partners in the consortium: Statistical and Communications Signal Processing

[1] SMARAD CoE, Signal Proc. Lab, Helsinki Univ. of Technology, PL 3000, FI-02015, TKK, Finland
[2] SMARAD CoE, Radio Lab, Helsinki Univ. of Technology, PL 3000, FI-02015, TKK, Finland
[3] Telecommunications Lab., University of Oulu,

research group, Principal Investigator Prof. Visa Koivunen and High Frequency and microwave engineering group, Principal Investigator Prof. Pertti Vainikainen.. The research group of Prof. Vainikainen has a strong background channel measurements and modeling as well as building antenna arrays. The research group of Prof. Koivunen has a strong background in smart antenna theory and algorithms , MIMO systems and statistical and array signal processing.

1.2 Telecommunication Laboratory, University of Oulu

The Telecommunication laboratory at the University of Oulu is among the leading laboratories in spread spectrum research and it plays an important role in product development for many Finnish companies.
The SMAS group (Smart Antennas and Systems for future mobile communications) of Prof. Erkki Salonen from University of Oulu is the third partner in the MACMOT consortium. The research group of Prof. Salonen has a strong background in channel modeling and antennas. The group is a part of Infotech Oulu.

1.3 Funding

Table 1. Funding of the project in 1000 EUR in 2003-2006. Internal funding consists of manpower costs and operational expenditures provided by the organisation. The funding from Academy is used for salaries. Funding for equipment needed for building test bed and measurement systems is acquired from different sources.

Partner	Funding organisation	2003	2004	2005	2006	**Total**
TKK	Academy	31	67	67	46	**211**
UO	Academy	24	52	50	34	**160**
Total		**55**	**119**	**117**	**80**	**371**

In terms of person months, the effort in University of Oulu corresponds to 18 pmon/year and the effort in Helsinki University of Technology 24 pmon/year.

2 Research Work

The research work is subdivided into three workpackages:
-Developing optimised adaptive antenna configurations and their evaluation,
-Developing signal processing techniques small multiantenna configurations in mobile terminals, deriving optimal signal processing methods for arbitrary array configurations, dealing with array imperfections
-Testing of Adaptive Antenna and MIMO Systems

The objectives, technical rationale and key research problems and results are described in the following subsection.

2.1 Objectives and Work Plan

The goal of the project was to develop adaptive multiantenna systems for mobile terminals. Multiple antennas are needed because future multi-radio mobile terminals may have over 10 radios, each needing an antenna or antennas. Moreover, multiantenna systems in both base stations and mobile terminals lead to MIMO systems. Such systems provide a robust way to significantly improve spectral efficiency (bits/s/Hz) as well as the reliability of a radio link. Improvement in spectral efficiency is linearly related to the minimum number of transmit and receive antennas. MIMO is the key technology in future beyond 3G and 4G wireless communication systems, where data rates may be up to 1Gbit/s. Multiple antennas in a a mobile terminal tend to occupy plenty of space. Due to the small size of mobile terminals and other implementation constraints, multiple antennas have become a feasible option only recently. In an electrically small device, the whole structure contributes to the radiated power making the antenna design complicated.

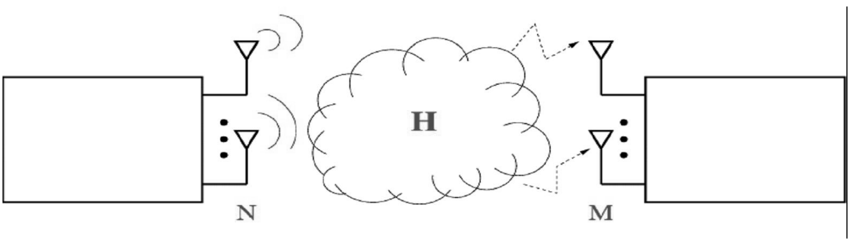

Figure 1. MIMO system for improving spectral efficiency and radio link reliability.

Availability of new small size antennas, advances in multidimensional propagation modeling, availability of MIMO channel measurements, deployment of higher frequencies, development of MIMO communication theory and diversity techniques have made the use of multiple antenna in a terminal very attractive. New antenna configurations that occupy less space and yield similar diversity and array gains have to be developed. In addition, new smart antenna techniques for arbitrary antenna configurations have been derived that possess desirable optimality and robustness properties. Low computational complexity and low power consumption are additional design goals for such methods. Availability of extensive propagation channel measurements facilitates creating experimental calculation-based antenna system test-bed where measured and simulated antenna patterns may be compared. In addition, performance tests using 3-D measurement system may be conducted in an anechoic chamber.

2.2 Common Themes and Collaboration

The workpackages are all solving parts of same problem of designing and evaluating multiantenna systems for mobile terminals. The collaboration was natural since every part of the project is in the same food chain. For example, the antenna measurements made in test bed systems were needed in computing the EADF. The resulting EADF is needed then in smart antenna algorithms used in a mobile terminals. Similarly, the performance of MIMO configurations and transceiver structures need to be evaluated using realistic propagation environments and multiantenna configurations.

The workpackages were also cooperating by sharing and exchanging antennas and measured propagation data as well as participating in the actual measurements. Close co-operation between antenna designers, propagation measurement people and antenna array/transceiver signal processing people has lead to world class theoretical research results

The co-operation was arranged in the context of joint meeting in the context of conferences and workshops such as COST 273, URSI and EuCAP meetings. Moreover, internal research seminars were organized where different workpackages presented their results. The discussions were lively and very informative for the participants. Obviously, the doctoral students have been also working in a practical level since they have been using the same antennas and measured propagation and calibration data.

2.3 Optimized adaptive antenna configurations and their evaluation

The new adaptive multi-antenna systems like MIMO (Multiple Input Multiple Output) antenna configurations are been predicted to provide significant improvement in the data transfer capacity of mobile radio links. However, especially in the mobile terminal there are significant limitations for the implementation of the multi-antenna structures. Due to the complicated propagation channel the prediction of the performance of the antenna system is difficult and requires thorough knowledge of the propagation channel. In this subproject the goal was to develop a new computational testbed to evaluate MIMO antenna structures and develop with the help of the testbed synthesis principles of optimal antenna configurations. In further work the testbed can also be used for testing adaptive algorithms thus enabling their evaluation with realistic time-domain propagation channels. The personnel involved this task were prof. Pertti Vainikainen, Pasi Suvikunnas, Juha Villanen, Veli-Matti Kolmonen.

The workpackage was divided into three tasks, whose main results are described below.

Establishment of the testbed (Suvikunnas)

In this task the computational measurement-based antenna testbed (MEBAT) for adaptive antennas was created based on existing 2 GHz propagation data. The idea of the testbed is described in Figure 1. The propagation data obtained from multi-dimensional (amplitude, directions, delay, polarization) propagation measurements through parameter extraction (see Task …tähän viite teidän työhön) is combined with the simulated or measured radiation patterns of the multi-antenna structure. This enables testing of arbitrary realistic antenna configurations without limitations of antenna patterns or number of elements. Furthermore, the method provides the possibility to change the orientation of the antenna, which is important for testing of mobile terminal antennas as their orientation is quite random in real use.

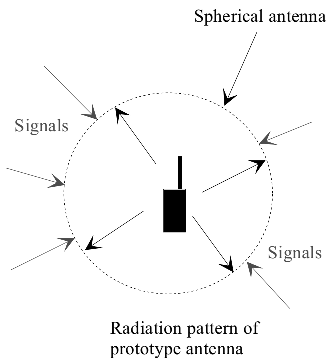

Figure 2. The principle of the antenna testbed.

In this project the accuracy of MEBAT was evaluated and it was discovered appropriate for evaluating both diversity and MIMO antenna configurations. This enabled antenna testing at 2 GHz frequency range for 3rd generation mobile terminals and also gave basis for further development of the testbed.

Extension of the testbed (Kolmonen, Suvikunnas)

In this task the basis of the testbed was extended with new 5 GHz MIMO measurements. They both provided a new frequency range for testing antennas of future mobile communications systems and also extended the testbed to full double-directional testing of arbitrary multi-antenna configurations at both ends of the link. In Figure 2, new antennas developed in this project for 5 GHz propagation measurements and an example of outdoor urban propagation data are shown. With the extended version of MEBAT it is possible to test both traditional basestation-to- mobile scenarios and also new mobile-to-mobile links, which have been studied extensively recently in theory by many research groups. In very recent work in this project mobile-to-mobile links have been studied experimentally by using the extended version of MEBAT.

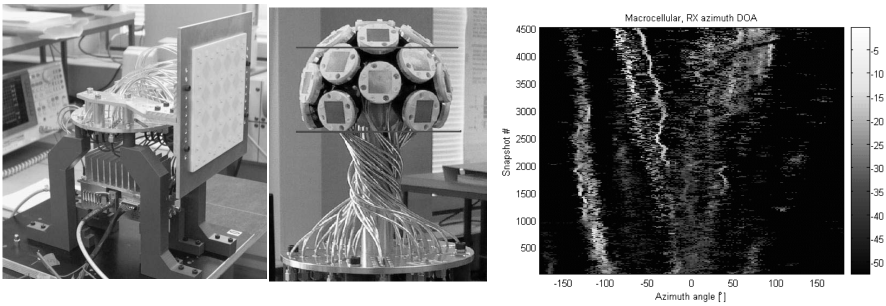

Figure 2. Antenna arrays for propagation measurements at 5 GHz (left) and direction-of-arrival distribution in a city street environment (right).

Antenna configuration synthesis (Villanen, Suvikunnas)

The performance of several mobile terminal antenna structures has been evaluated with MEBAT both at 2 and 5 GHz to find out features that are important for a multi-antenna configurations. In the study, implementation limitations of realistic antenna structures like those caused by small size, mutual coupling and low allowed complexity were taken into account and their effect was considered. In Figure 3 an example of comparison of antenna configurations is shown. The used evaluation criterion is the outage capacity for a MIMO system having the evaluated antenna configuration in the mobile. Also the effect of the user hand and head is included in the evaluation.

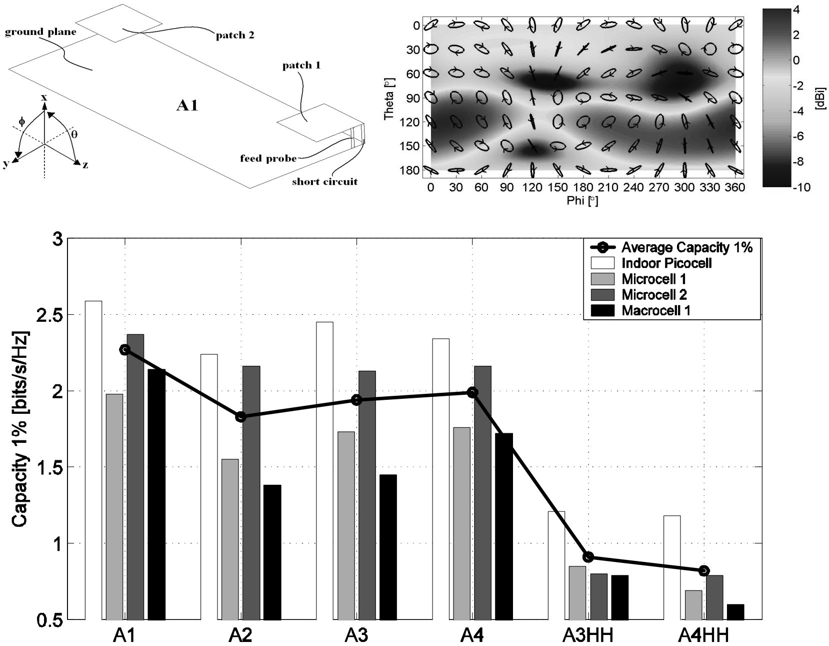

Figure 4. An example of a test prototype of a dual-antenna system for a small (100 x 40 mm^2) mobile terminal (top left), the simulated radiation patterns of the antenna elements (top right), and the 1% outage capacity obtained for four different antenna structures in free space (A1-A4) and for two of them beside a human head and hand model (A3HH and A4HH).

2.3 Developing optimal signal processing methods for multiantenna configurations in mobile terminals

In this work we have developed antenna array techniques for arbitrary array configurations. This is an important issue when designing handheld terminals equipped with multiantenna transceivers. Optimal antenna array techniques are typically derived for a uniform linear array (ULA). In mobile terminals no such regular array structure can be used because of small space, other components (e.g., processors, display, keyboard, speaker, camera) in the platform, aesthetic design requirements. Moreover, the whole chassis is serving as an antenna causing many imperfections such as mutual coupling. Therefore, it is important to derive optimal array processing techniques that may be used in arbitrary array configurations. The personnel involved with this workpackage were doctoral student Fabio Belloni, Dr. Andreas Richter and prof. Visa Koivunen.

In this work we derived a manifold separation technique (MST), which stems from the wavefield modelling formalism developed for array processing. MST is a method for modelling the steering vector of antenna arrays of practical interest with arbitrary 2-Dor

3-D geometry. It is the product of a sampling matrix (dependent on the antenna array only) and a Vandermonde structured coefficients vector depending on the wavefield only. This allows fast array processing (e.g. Direction-of-Arrival (DoA) estimation, beamforming, space division multiplexing) algorithms designed typically for linear arrays to be used on arrays with arbitrary configuration. MST does not require any subdivision into angular sectors and provides many orders of magnitude smaller error than any array interpolation technique.

The method uses the calibration data and in particular its inverse discrete Fourier transform (IDFT) to create so-called effective aperture distribution function (EADF). This technique also takes into account the array imperfections since they are present in the calibration data. Morover, any type of beampatterns of individual array elements can be handled. The IDFT is commonly truncated to get the final EADF.

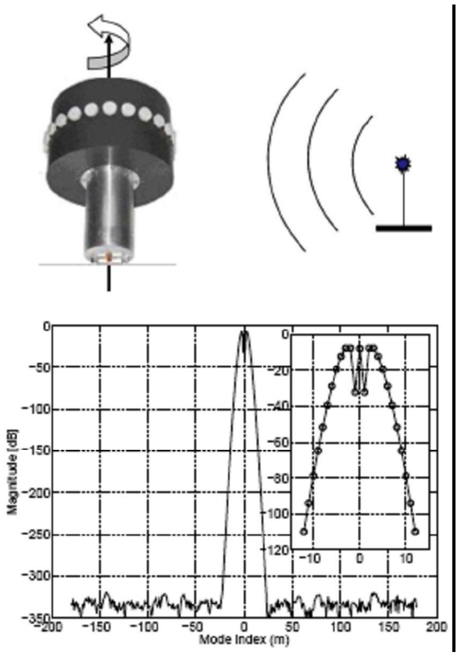

Figure 5. Acquiring calibration data and magnitude of array characteristics of one element.

Let us consider direction finding as an example application. Mobile terminal user could track some other phone user or a pet carrying a beacon. By employing EADF, one could find the angle of arrival of the signal with very high precision with low complexity (based on polynomial rooting). Moreover, the performance close to theoretical Cramer-Rao Lower bound despite the array imperfections would be achieved. A high-level block diagram of the direction finding is presented in Figure 6.

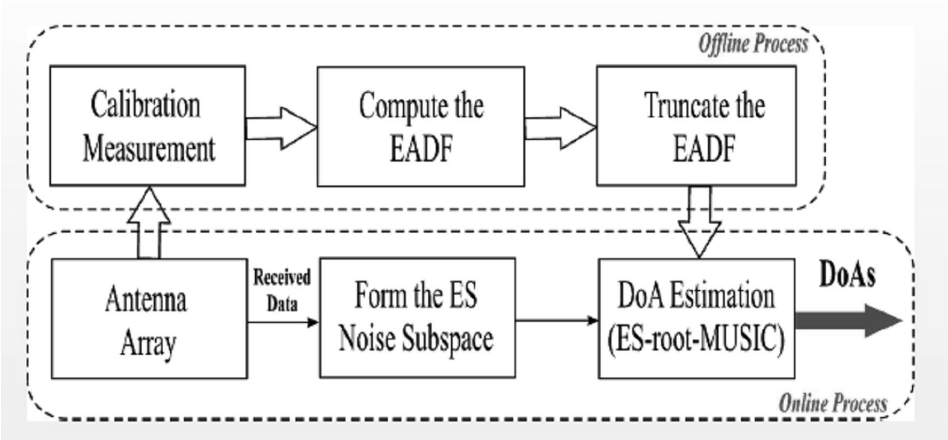

Figure 6: Stages in low-complexity direction finding for arbitrary array configurations.

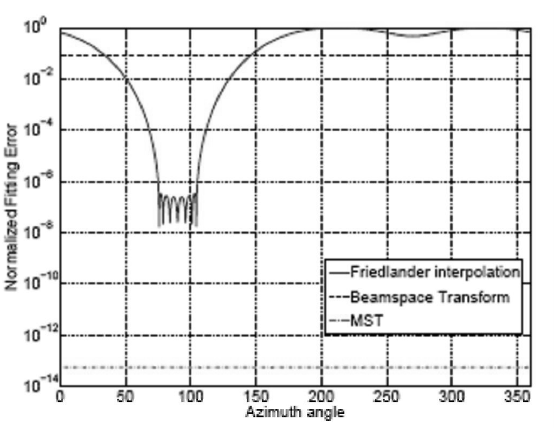

Figure 7: Error magnitudes for array interpolation and MST techniques. The error in MST is extremely low i.e. in machine precision level.

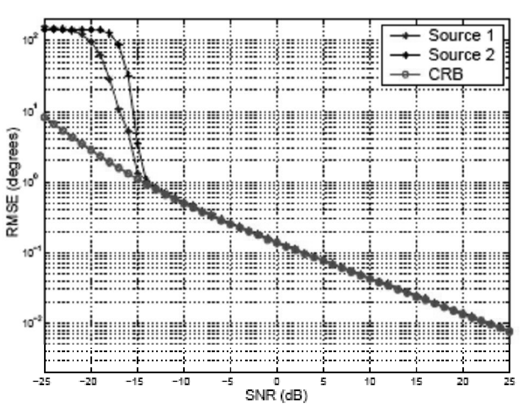

Figure 8: Direction finding performance in two user (or multipath) case.

In real-world applications, the calibration measurements used to determine the sampling matrix are corrupted by noise. This impairs the performance of MST-based algorithms. We have studied the effect of noisy calibration measurements on subspace-based DoA analytically and in simulation. Mathematical expressions for the error have been established. Tecnique has also been applied to real-world arrays depiced in Figure 8.

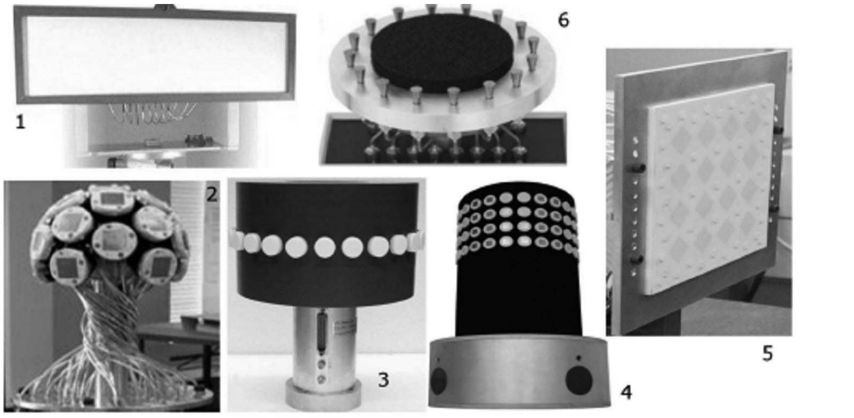

Figure 9: Real world arrays used in this study.

Just to conclude in this workpackage techniques for using optimal and low-complexity smart antenna techniques in small multiantenna terminals were developed. This allows using optimal array processing techniques in arbitrary array configurations. Such configurations are unavoidable immobile terminals because of numerous design constraints.

2.4 Development of three dimensional measurement system for performance tests of adaptive antennas and MIMO systems

One problem for adaptive antenna development is to test its performance. A 3D-measurement system for adaptive antenna systems in the anechoic chamber of the University of Oulu is designed. The idea of the 3D-measurement system is to simulate wanted (line-of-sight and multipath components) and unwanted (interference) radio signals from different directions. In the tests of adaptive antennas, signals from each antenna element are stored synchronously and these data can be used for testing different adaptive algorithms in reproducible conditions. The designed 3D-measurement system consists eight transmitter antennas, which can be placed in different locations in the anechoic chamber. Each transmitter antenna can be used to simulate one radio path of the wanted signal or interference signal. This environment, one of the firsts of its kind, constitutes a systematic acquisition system and data base for 3D-radiation effects in cellular systems. The system is planned for frequencies from 1 to 7 GHz. Therefore, it covers frequency bands used in 3G-cellular systems, most WLAN-systems and possibly future 4G systems. It can be configured also for MIMO system validation.

Two alternative receiver configurations were considered: parallel synchronous channel and time division multiplexing. By using time-division multiplexing at the receiver, the PropSound™ channel sounder, made by Elektrobit Group, was used to demonstrate the system. Eight elements uniform circular array (UCA) was used as a receiving antenna when two antennas were used as transmitting antennas. UCA was moved on turntable using different measurements setups. The demonstration results using PropSound™ are promising but more detailed post processing is still needed. Results can be seen after post processing by using DOA and beamforming algorithms. Calibration matrix used in DOA algorithm is created from the measured data. DOA algorithm used was MUSIC (Multiple Signal Classification). Based on the demonstration, more economical time-division multiplexing receiver system is implemented.

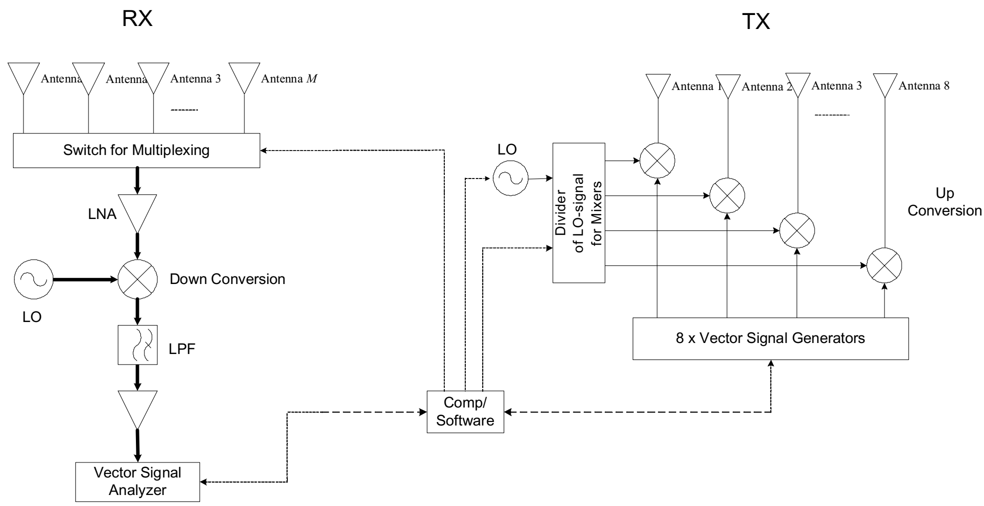

Figure 10: Multiantenna Measurement System

Antenna array research

Several antenna arrays for mobile communications are designed, simulated, fabricated and measured. Mutual coupling effects between different elements were also studied. Antenna size is a very important parameter in antenna element design for mobile terminals. Ceramic materials and frequency tunable antennas are studied for antenna miniaturization. Results are published in Master Thesis and conference papers.

Partially based on the expertice achieved in this project, a new research project ”Future Active Multiband Antennas” in TEKES ELMO-program was started in 2005. It focuses on the research and development of actively tuned, miniature multiband antennas. This research is carried out in collaboration with the Telecommunication Laboratory and the Microelectronics and Material Physics Laboratories at University of Oulu. Based on these two research projects, an active antenna research team has formed in the University of Oulu.

3 International Aspects

The project participants were actively contributing to European COST 273 project in the areas of antenna design and propagations studies. The network of partners through that project is very large, Moreover, there has been co-operation with Ilmenau University of Technology in the areas of propagation and antenna measurements as well as channel modeling based on estimated propagation parameters. There has been numerous researcher exchanges between the TKK and Ilmenau from a few days up to several months. Other international research partners are University of Bologna and University of Nice where prof. Pertti Vainikainen spent a mini-sabbatical in summer 2006.

4 Publications and Academic Degrees

In terms of academic degrees the outcome of the project looks as follows:
Doctoral degrees: Pasi Suvikunnas (2006), Fabio Belloni (expected 2Q/2007), Juha Villanen (expected 3Q/2007); *Licentiate Degrees*: Veli-Matti Kolmonen (1Q/2007); *M.Sc. Degrees*: Marko Sonkki, Jarkko Peltonen, Jukka Kyröläinen, Esa Ylitalo

In terms of scientific publications the project has produced *9 journal papers*, *25 conference papers*, 10 COST 273 documents. Dr. Andreas Richter and prof. Visa Koivunen co-authored papers receiving the best paper awards in European Signal Processing Conference (EUSIPCO 2006), and European Conference on Antennas and Propagation (EuCAP 2006).

Table 2. Publications and academic degrees produced in the project. Numbers of different types of publications are given along with the reference numbers. List of refereed journal articles are given in Section 6.1, refereed conference papers in Section 6.2, monographs in Section 6.3 and theses in Section 6.4.

Partner	Type of publication	2003	2004	2005	2006	**Total**	Publication numbers
TKK	Ref. journal art.					**9**	
	Ref. conf. papers					**22**	
	Monographs	-		-	-		
	Doctoral dissert.				-	**3**	(2 of them expedted)

	Licentiate degrees	-		-	-	**1**	(expected)
	Master degrees						
UO	Ref. journal art.					**1**	
	Ref. conf. papers					**3**	
	Monographs		-	-	-		
	Doctoral dissert.				-		
	Licentiate degrees		-	-	-		
	Master degrees					**6**	

5 Other Activities

Here the project reports on other activities, such as consortium kick-off meetings and steering activities, arranged conferences and seminars, joint meetings of the participating groups, and activities for dissemination of results including popularised presentations on their research work.

6 Publications

6.1 Refereed Journal Articles

1. K. Sulonen, P. Suvikunnas, L. Vuokko, J. Kivinen, P. Vainikainen, “Comparison of MIMO antenna configurations in picocell and microcell environments”, *IEEE Journal on Selected Areas in Communications* vol. 21,no. 5, June 2003, pp. 703- 712.

2. J. Villanen, J. Ollikainen, O. Kivekäs, and P. Vainikainen, "Coupling element based mobile terminal antenna structures", *IEEE Transactions on Antennas and Propagation*, vol. 54, no. 7, July 2006, pp. 2142- 2153.

3. V.-M. Kolmonen, J. Kivinen, L. Vuokko, and P. Vainikainen, ” 5.3 GHz MIMO radio channel sounder”, *IEEE Transactions on Instrumentation and Measurement*, vol. 55, no. 4, August 2006, pp. 1281- 1287.

4. P. Suvikunnas, J. Villanen, K. Sulonen, C. Icheln, J. Ollikainen, and P. Vainikainen “Evaluation of the performance of multi-antenna terminals using a new approach,” *IEEE Transactions on Instrumentation and Measurement*, vol. 55, no. 5, Oct. 2006, pp. 1804 - 1813.

5. P. Vainikainen, P. Suvikunnas, and L. Vuokko, “Experimental performance evaluation of MIMO antenna configurations in indoor environments at 5 GHz frequency range”, accepted for publication in *Proceedings of the European Microwave Association*, vol. 2, no. 3, 2006.

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10. Komulainen M., Mähönen J., Tick T., Berg M., H. Jantunen, M. Henry, C. Free, E. Salonen: Embedded air cavity backed microstrip antenna on an LTCC substrate, Journal of European Ceramic Society, (accepted for publication)

6.2 Refereed Conference Papers

1. K. Sulonen, P. Suvikunnas, J. Kivinen, P. Vainikainen, “Study of different mechanisms providing gain in MIMO systems”, *Proceedings of the 58th IEEE Vehicular Technology Conference VTC Fall 2003*, Orlando, Florida, USA, October 6-9, 2003.

2. J. Villanen, P. Suvikunnas, C. Icheln, J. Ollikainen, P. Vainikainen, “Advances in diversity performance analysis of mobile terminal antennas”, *International Symposium on Antennas and Propagation (ISAP)*, Sendai, Japan, 17.-21.8.2004. Sendai, Japan 2004, The Institute of Electronics, Information and Communication Engineering, paper 3A3_3.pdf.

3. P. Vainikainen, J. Villanen, K. Sulonen, P. Suvikunnas, J. Ollikainen, “Antennas for future mobile terminals”, *2004 Asia Pacific Microwave Conference*, New Delhi, India, December 15-18, 2004. New Delhi, India 2004, paper no 642, 5p. (invited).

4. P. Vainikainen, K. Sulonen, J. Kivinen, P. Suvikunnas, L. Vuokko, J. Salo, V.-M. Kolmonen; X. Zhao, H. El-Sallabi, “Experimental MIMO propagation modeling and antenna system evaluation”, *IEEE AP-S International Symposium*, Monterey, CA, USA, June 20-26, 2004, file s048p12a.pdf (invited).

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10. J. Salo, P. Suvikunnas, H. El-Sallabi, P. Vainikainen, "On the distribution of capacity in rayleigh fading MIMO channels", *Nordic Radio Symposium*, Oulu, Finland, August 16-18, 2004. Oulu, Finland 2004, TUEAM1_1.pdf.

11. J. Salo, P. Suvikunnas, H. El-Sallabi, P. Vainikainen, "On the characteristics of MIMO mutual information at high SNR", *6th IEEE Nordic Signal Processing Symposium*, Espoo, Finland, June 9-11, 2004. 78_SALO.pdf.

12. V.-M. Kolmonen, J. Kivinen, L. Vuokko, P. Vainikainen, "5.3 GHz MIMO radio channel sounder", *IEEE Instrumentation and Measurement Conference IMTC'05*, Ottawa, Ontario, Canada, May 16-19, pp. 1883-1888.

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15. J. Salo, B. Badic, P. Suvikunnas, H. Weinrichter‡, M. Rupp, and P. Vainikainen, "Performance of space-time block codes in urban microcells: the effect of antennas", *The 8th International Symposium on Wireless Personal Multimedia Communications (WPMC'05) Proceedings*, Aalborg, Denmark, 18-22 Sept, 2005, pp. 1848-1852.

16. L. Vuokko, P. Suvikunnas, J. Salo, J. Kivinen, P. Vainikainen, "Comparison of measurered MIMO capacities at 2 and 5 GHz," *XXVIIIth General Assembly of URSI*, New Delhi, India, 22-29 October, 2005, pp. 1-4 (invited).

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6.3 Monographs

6.4 Doctoral, Licentiate, and Master Theses

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Ylitalo E.: Wideband small antenna design and their radiant efficiency measurements, , Univ. of Oulu, Master´s Thesis, (in finnish) 2006

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J. Kivinen, P. Suvikunnas, J. Salo, P. Vainikainen, ”Effect of antenna polarization in 2x2 MIMO system”, *COST273 Temporary Document*, TD(03)197, Prague, Czech Republic, Sept. 2003, 6 p.

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P. Suvikunnas; J. Salo, J. Kivinen,; Vainikainen, Pertti, *A figure of merit for MIMo antenna evaluation*, Athens, Greece, COST 273-Temporary Document TD (04)032.

P. Vainikainen, “Advances in measurement and estimation methods”

ULTRA LOW-POWER VIDEO COMPRESSION SYSTEM FOR MOBILE DEVICES

Professor Ari Paasio[1]

Abstract

In this work research efforts were targeted towards a design of low-power video compression system. The aim was to achieve a compression system where the key blocks are realized using analog circuits, thus resulting lower power consumption than digital realizations. The motion estimation is responsible for being the most power hungry part in the encoder. The design of this block in our approach was based on novel motion estimation algorithm where the power consumption of the particular DCT evaluation block was the figure of merit and the least power hungry block was selected as the winner. Unfortunately, only comparable results to conventional SAD based search were achieved. An AD converter was designed with built in quantization capability to convert the analog DCT results into digital domain. Also, some methods of improving the inherent inaccuracy of analog computation in an algorithmic level were investigated. Hardware tuning for accuracy was found to be important also in this work and the research was directed towards two different approaches, namely to floating gate tuning and to combination selection. Floating gate operation is very challenging in current technologies with thin gate oxides where on the other hand, combination selection utilizes the randomness of minimum area transistors. Thus, the combination selection would at this point of research seem to be a good candidate for accuracy tuning in nano scale devices that are inherently very inaccurate. Different building blocks were designed and sent to fabrication, after which they were evaluated and also reported in various forums.

1 Partners and Funding

1.1 Microelectronics Laboratory, University of Turku

The research group consists of project leader professor Paasio, Dr. Mika Laiho and postgraduate students Mr. Mikko Pänkäälä, Ms. Kati Virtanen (1.1.2005 – 31.4.2005, 1.5.2005– GETA graduate school) and Mr. Janne Maunu (1.5.2005–). In supporting activities there are postgraduate students Mr. Jonne Poikonen (PhD Dec 2006), Ms. Laura Vesalainen, Mr. Joona Marku, doctor Pasi Liljeberg and professor Juha Plosila.

The laboratory was founded in 2003 when Ari Paasio started as a professor at the University of Turku (UTU) and the project joined the TULE program in 2005 in a second application round targeted for circuits and systems research.

[1] Microelectronics Laboratory, University of Turku, Joukahaisenkatu 3-5, FIN-20520 Turku

1.2 Funding

Table 1. Funding of the project in 1000 EUR in 2003-2006. Internal funding consists of manpower costs and operational expenditures provided by the organisation. The funding provided by the Academy of Finland and other external sources is also shown in the table.

Partner	Funding organisation	2003	2004	2005	2006	**Total**
UTU	UTU	12	32	5	15	**64**
	Academy	0	0	64	56	**120**
	Academy (GETA)	0	0	16	24	**40**
Total		**12**	**32**	**85**	**95**	**224**

2 Research Work

2.1 Objectives and Work Plan

The **first goa**l was to develope a motion estimation system that is highly parallel and uses results of multiple Discrete Cosine Transform (DCT) blocks in the best matching block search process.

The **second goal** of this project was to develop, apply and demonstrate a design method for implementing mixed analog/digital circuits by using asynchronous design approach. We believe it is one of the most promising approaches to make a significant step in the power consumption reduction as well as to obtain low noise characteristics of integrated mixed signal circuits.

Current-mode signaling is used in our analog processing blocks to meet the strict speed requirements and to get rid of area consuming capacitors. Our strategy was to do the AD-conversion as late as possible to get the maximal benefit out of smaller and more efficient analog building blocks. The development of a dedicated AD-converter structure with an adaptive quantization scheme is our **third goal**.

One of the most challenging task in architectural level is minimizing the memory I/O. Especially motion estimation requires large amount of intermediate results to be stored in memories. Storing only essential data in the right form is crucial from the power consumption point of view. At this point we have several options how to solve this problem. The **fourth goal** was to make advances in the intelligent memory accessing.

In the progress of the project it became apparent that the accuracy of analog computation is of highest importance in video compression. Therefore, the project was redirected towards finding a way to tune the analog accuracy with competitive layout area (**NEW GOAL**). Two approaches were considered, namely a floating gate tuning or a combination selection. The redirection of the project was done at the cost of abandoning the original fourth and second goal.

2.3 Final Report

This project as well as the hosting laboratory is very young, but encouraging progress has been achieved although many ideas have turned out not to offer major break throughs as originally expected by the project. The ideas have, however been evaluated, and can be further developed in video compression application in particular or in other analog signal processing devices.

Test structures (integrated circuit, 0.25 micron CMOS technology) designed by Mr. Pänkäälä for his M.Sc. on analog DCT cores [3] has been measured and a journal article based on these results has been published [1]. A new measure for DCT-based motion estimation was developed where the winning candidate was selected on the basis of minimum power supply usage. However, this approach yielded only comparable results to simple SAD based selection as far as the rate-distortion measure is concerned. This lead a need to furter develop the original analog DCT core, but no good candidates have been found so far.

Test chips for the AD-converter designed by Ms. Kati Virtanen have been measured and reported in [5] and in [8]. The designed AD converter gets its input from an analog DCT block whose result is rectified by the circuit reported in [2].

Also, a test chip (130nm CMOS) including test structures for floating-gate tuning have been evaluated and findings are being reported in e.g. [11]. These particular test structures were designed by Mr. Pänkäälä and Dr. Laiho. Floating gate results are also reported in [4].

New ideas also in the mismatch compensation by combination selection have been evaluated. One such method is reported in [7] and in [10]. System level MATLAB simulation environment with analog computation mismatch models is currently being developed and applied to various research areas within the laboratory. Some findings on DCT mismatch compensation are reported in [6]. A special digital counter [9] has been designed, where the main effort has been in another project but the results are applicable to video compression also.

3 International Aspects

Mr. Pänkäälä attended a three week Telluride workshop (http://ine-web.org/telluride-conference-2006/telluride-overview/index.html) in the summer of 2006 where the participants are within the top academic research laboratories in the world working in the areas of intelligent imagers, analog image processing (including floating gate usage in DCT by group of professor Hasler, Georgia Tech, USA) and robotics. Our group now participated to this workshop for the second time, where Dr. Laiho participated in 2005.

4 Publications and Academic Degrees

Table 2. Publications and academic degrees produced in the project. Numbers of different types of publications are given along with the reference numbers. List of refereed journal articles are given in Section 6.1, refereed conference papers in Section 6.2 and theses in Section 6.3.

Partner	Type of publication	2003	2004	2005	2006	**Total**	Publication numbers
UTU	Ref. journal art.	-	-	-	1	**1**	1
	Ref. conf. papers	1	2	2	5	**10**	2-11
	Monographs	-	-	-	-	**-**	
	Doctoral dissert.	-	-	-	-	**-**	
	Licentiate degrees	-	-	-	-	**-**	
	Master degrees	2	-	-	-	**2**	12-13

5 Other Activities

Professor Paasio presented the project in Helsinki at the event organized by the Academy of Finland and directed to the Finnish press in July 2006.

6 Publications

6.1 Refereed Journal Articles

[1] M. Pänkäälä, K. Virtanen and A. Paasio, An Analog 2-D DCT Processor, IEEE Transactions on Circuits and Systems for Video Technology **16** (2006) 1209-1216.

6.2 Refereed Conference Papers

[2] J. Poikonen, A. Paasio, “An Area-Efficient Full-Wave Current Rectifier for Analog Array Processing”, ISCAS 2003, Bangkok, Thailand, 2003.

[3] M. Pänkäälä, J. Poikonen, L. Vesalainen, A. Paasio, “Realization of an Analog Current-Mode 2-Dimensional DCT”, ISCAS 2004, Vancouver, Canada, 2004.

[4] M. Pänkäälä, A. Paasio, M. Laiho “A Floating-Gate Approach for Obtaining Accurate Current References in the CNN”, the 8^{th} International Workshop on Cellular Neural Networks and their Applications, Budapest, Hungary, 2004.

[5] K. Virtanen, M. Pänkäälä, A. Paasio, “A Current-Mode ADC with Adaptive Quantization”, ISCAS 2005, Kobe, Japan, 2005.

[6] K. Virtanen, M. Pänkäälä, A. Paasio, “Compensation of Errors Generated by an Analog 2-D DCT”, ISCAS 2005, Kobe, Japan, 2005.

[7] J. Maunu, M. Pänkäälä, J. Marku, J. Poikonen, M. Laiho, A. Paasio, “Current Source Calibration by Combination Selection of Minimum Sized Devices”, ISCAS 2006, Kos, Greece, 2006.

[8] K.Virtanen, M. Pänkäälä, M. Laiho, A. Paasio, “Implementation of an Asynchronous Current-Mode ADC with Adaptive Quantization”, ISCAS 2006, Kos, Greece, 2006.

[9] J. Marku, M. Pänkäälä, J. Plosila, A. Paasio, "Combination Selection Counter for Gaussian Distribution Applications", MWSCAS 2006, San Juan, Puerto Rico, 2006.

[10] J. Maunu, J. Marku, M. Laiho, A. Paasio, "An On-Chip Measurement Circuit for Calibration by Combination Selection", IEEE International SOC Conference, Austin, Texas, USA, 2006.

[11] M. Pänkäälä, M. Laiho, A. Paasio, "Experiments with Floating Gate Devices in 0.18 and 0.13 Micron CMOS Technologies", NORCHIP 2006, Linköping, Sweden, 2006.

6.3 Doctoral, Licentiate, and Master Theses

[12] M.Pänkäälä, Realization of an Analog Current-Mode 2-D Discrete Cosine Transform, Masters thesis, Department of Information Technology, University of Turku, 2004.

[13] K. Virtanen, DCT Error Compensation and A/D Conversion with Adaptive Quantization, Master thesis, , Department of Information Technology, University of Turku, 2004.

WIRELESS PHYSIOLOGICAL SENSORS FOR AMBULATORY AND IMPLANTABLE APPLICATIONS

Jukka Lekkala[1], Jari Hyttinen[2], Markku Kivikoski[3], Jukka Vanhala[3], and Minna Kellomäki[4].

Abstract

An implantable ECG-measurement device was mainly under research interest. General effects of implantation on measurement sensitivity were modeled, and thus the signals measured from implanted electrodes can be predicted. The results of these studies indicated that implanting the measuring electrodes under the skin has minor effect on the measurement sensitivity compared with implanting the electrodes under the costals or even on the heart muscle. The characteristics of electrodes and electrode materials for implantable ECG-measurement system were studied. Silver (Ag), silver-silver chloride (Ag/AgCl), and platinum (Pt), stainless steel (SS) and gold (Au) together with several different electrolytes were tested. SS was proven to be one of the best materials to be used as an implantable electrode.

Few prototypes of an implantable electrocardiography measurement system were designed and implemented. The measurement system is divided into two parts: the transponder and the reader. Inductive coupling is used in bidirectional data transfer between the reader and the transponder. Magnetic fields generated by the reader are also used for transferring power to the transponder making the implantable device passive. The feasibility of ultrasonic-based energy transmission into an implantable device was studied both on the basis of ultrasonic theory and demonstrative measurements. Due to difficult implementation in real life measurement situation, the ultrasonic transponder was not implemented into the measurement device. Different packaging techniques suitable for implantable devices have been studied. Since the device needs maximum miniaturisation, flip chip technique has been the focused technology. Joining has been done using anisotropically conductive adhesive, which only conducts in z-direction. Also the effect of different coatings and sterilization is under study. Reliability testing has been done according to standard JESD22- A101-B, where temperature is 85 °C and relative humidity 85 %. One test lasts 1000 hours. Failure mechanisms will be analyzed with optical microscopy and scanning electron microscopy.

Selection, processing and testing of coating material, especially polymers for the enclosure of implantable sensor and measuring system, were performed. The basic coating material was chosen to be epoxy which was further coated with a few micro meters thick parylene-C coating. The experiments and literature both favored this type of coating method. An extensive research was made on the standardization and legal part of the design process of an implantable device. ISO 9001, ISO 13485, and FDA Design Control Guidance were revised and summarized. Passive wireless, subcutaneous devices were also studied. Laboratory prototypes of these devices relied on an LCR-resonator that could be read from a short distance. Either L, C or R was held as variable and the resonance frequency revealed the value of the unknown component. During the project two in vivo tests were performed with the implantable ECG-measurement devices. Both of these tests were performed in cows in Finland. The first experiment was successful, in the second there were some problems in acquiring the signal from the cow.

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[3] Institute of Electronics, Tampere University of Technology, P.O. Box 692, FIN-33101 Tampere

[4] Institute of Biomaterials, Tampere University of Technology, P.O. Box 589, FIN-33101 Tampere

1 Partners and Funding

The partners of our **Wireless Sensing Consortium** and summary of funding are reported in the following:

1.1 Institute of Measurement and Information Technology, Tampere University of Technology

The research group consists of project leader professor Jukka Lekkala, postgraduate student Jarno Riistama (9/2003 – 2006) and students Janne Kiilunen (6 - 8/2004) and Tuula Lahna (5/2005 – 9/2006).

1.2 Ragnar Granit Institute, Tampere University of Technology

The research group consists of subproject leader professor Jari Hyttinen, postgraduate student MSc Juho Väisänen (10/2003 – 12/2006) and student Milla Ylinaatu (11/2004 - 04/2006).

1.3 Institute of Electronics, Personal Electronics, Tampere University of Technology

The research group consists of subproject leader professor Jukka Vanhala, senior researcher Jaana Hännikäinen (1/2004 – 12/2006, part-time), postgraduate students Sami Heinisuo (1/2004 – 7/2006) and Tomi Tieranta (5/2004 – 4/2005), Tero Häkkinen (6 – 8/2005) and Satu Arra (6/2004 – 12/2006).

1.4 Institute of Electronics, Microelectronics, Tampere University of Technology

The research group consists of subproject leader professor Markku Kivikoski, Docent Pekka Heino, and postgraduate students Kati Kokko (9/2003 – 12/2005) and Maunu Mäntylä (2006).

1.5 Institute of Biomaterials, Tampere University of Technology

The research group consists of subproject leader professor Minna Kellomäki and postgraduate students Anna-Maija Haltia (2003 – 2005) and Hanna Harjunpää (2005 – 2006). Students Hanna Harjunpää (2003 - 2005), Susanna Kumpulainen (2005 - 2006), and Sanna Peltola (2006, part-time).

1.6 Funding

Table 1. Funding of the project in 1000 EUR in 2003 - 2006. The funding provided by the Academy of Finland and other external sources is shown in the table.

Partner	Funding organisation	2003	2004	2005	2006	**Total**
TUT/MIT	Academy	20.4	49.5	54.1	32	**156**
TUT/RGI	Academy	23	39.5	53.1	57.4	**173**
	Private funds	0	10	1.5	15.5	**27**
TUT/ELE Personal el.	TUT/ELE	5	10	10	10	**35**
	Academy	22	53	53	33	**161**
TUT/ELE Packaging	Academy	21	54.6	53.4	32	**161**
TUT/BIOM	Academy	20	50	54	32	**156**
Total		**111.4**	**266.6**	**279.1**	**211.9**	**869**

On the basis of this "Wireless physiological sensors for ambulatory and implantable applications" project financed by the Academy of Finland a new research project titled as "Short-range wireless sensor platform for ambulatory and implantable applications" (WISEPLA) financed by Tekes and 11 Finnish companies started in the beginning of 2006. The project is carried out by our Wireless Sensing Consortium, and it continues with the work that has been started in the TULE programme. Total budget of the WISEPLA is 1.12 million euros for the years 2006 - 2008.

2 Research Work

2.1 Objectives and Work Plan

The aim of this project was to study and develop wireless sensor technology for ambulatory and implantable human psychophysiological applications. The wireless sensors were planned to be demonstrated in certain soft and hard tissue implant applications such as implantable electrodes for detection of cardiac state or bone implant monitoring. These applications have a high potential to be realized as commercial products. Thus, the applications give some good demonstration platforms without limiting the future use of the technology to be developed. The electronic integration and packaging technology provide tools to produce the measurement electronics and the telemetry systems into single chip size objects. This multilayer circuitry will include sensors, basic signal conditioning, analog-to-digital converters, embedded micro controllers and wireless communication electronics. The biomaterial and tissue engineering sciences provide tools to tailor biocompatibility and functionality of the surfaces of the implantable sensors. The developed prototypes were planned to be tested in vitro and additional in vivo animal studies may be possible to perform within other projects. The project was expected to produce new technology and knowledge for ambulatory and implantable human psychophysiological measurements. This includes the implantable measurement systems *per se*, transmission of data and power to and from implanted devices, the electric packaging of microsensors and measurement instrumentation for implantable application, and selection and testing the biocompatible coating material related to the implantable sensors. The planned demonstrations in this project were: 1) Implantable wireless electrocardiogram (ECG) device, and 2) Sensor implant for monitoring of closing the sternum after large thorax operations. In addition new innovative sensing challenges are studied for the following clinically important implants; a sensor system as part of hip prosthesis, and a wireless coronary stent sensor. The research of this project is based on combining the research efforts of five research groups having the necessary background.

The objective of microelectronics was to reduce the size and energy consumption of these packages by using 3D system-in-package (SiP) technology. Other objectives were the design of a hermetic package and study of long term reliability issues.

2.2 Final Report: Common Themes and Collaboration

One common theme of the research is the physical size and design of the implanted transponder. The size and shape have effect on the electrode size and inter-electrode distance. The electrode layout affects the sensitivity of the measurement and lead field in the heart. Thus, it is important that the modelling, electrode design and transponder device planning is made in a cooperative process.

Another common theme is the coating and protection of the transponder. It has effect on the miniaturization, electrode design and biocompatibility. Again, this theme binds several research groups together. The wireless link and inductive power delivery system set certain limits for the design and layout of the transponder and reader. The optimum solution for the given problem, how to measure ECG and heart rate by using a passive transponder type device, can be found only by a real collaboration.

Coating and wetting issues were studied in close collaboration with the Institute of Electronics and Institute of Biomaterials. Low power issues related to data and power transfer were collaborated with the packaging group and personal electronics group of the Institute of Electronics. Electrode material and joining issues were studied in collaboration with the Institute of Electronics and Institute of Measurement and Information Technology.

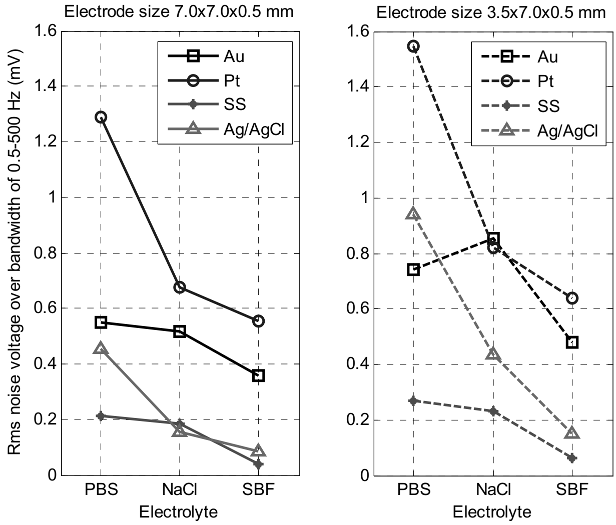
The whole project is based on intensive collaboration between the participating groups. All participating parties of the research have to be very familiar with the extremely complex environment where the device will be operating. The different research areas have completed each other and everyone that took part in the project has learned a lot about the different fields of research. When the research group was striving for a common goal, the decisions could be made by an individual researcher and still take into account the others. It was vital that everybody were conscious about the impact of their decisions on the whole project. The research groups have had common project meetings almost every week, and also several innovation meetings to promote new solutions. The project has a website (www.ele.tut.fi/TULE) which includes external pages to introduce our project and main results, and also internal pages for easy communication and report collection and delivery.

2.3 Progress Report: Progress by the Institute of Measurement and Information Technology

The Institute of Measurement and Information Technology has been working with the implantable ECG-measurement system and studied especially the characteristics of electrodes and electrode materials. The most suitable material for electrodes to be implanted into humans has been studied by using impedance, noise and corrosion measurements. The area and material of the electrodes have been determined based on this research. Platinum is showing the best performance and lowest noise according to [7] but new measurements with a broader range of materials indicate that stainless steel is also a good alternative [17]. Stainless steel (SS) is much cheaper material than platinum if one thinks a commercial product with high volumes.

The material research was done in [7] with a spectrum analyzer and an LCR-meter. Noise properties of materials were investigated first by manufacturing arrays of electrodes each containing three identical electrodes of the same material dipped into 0.9 m-% NaCl-solution (saline) electrolyte. Three electrodes needed to fulfill the measurement configuration required by the instrumentation amplifier: two electrodes to obtain the difference of random electrochemical noise between the two electrodes and the third one to provide a bias current path for the amplifier. The differential measurement signal was amplified by 13 dB to exceed the noise level of the amplifier. The measurement was made with a spectrum analyzer on the bandwidth of 2 - 500 Hz. The electrodes were allowed to stabilize in saline for one minute prior to measurement start. Materials that were investigated were silver (Ag), silver-silver chloride (Ag/AgCl) and platinum (Pt). Two different areas for the Ag and Ag/AgCl –electrodes were tested. Ag/AgCl –electrodes were made by chloridizing the Ag electrode with a 3 V positive voltage for two minutes which was determined to be enough to achieve a uniform layer of Ag/Cl on the electrode. The electrode-electrolyte interface impedance was measured with an LCR-meter at two frequencies, 120 Hz and 1 kHz. The measurements were performed in saline by dipping two electrodes of the same material and the same area into the solution. LCR-meter is able to distinguish the resistive and capacitive part of the interface impedance from each other.

A more wide research concerning the electrode characteristics was conducted in 2004-2005. Materials under research were Pt, stainless steel (SS) and gold (Au). Ag/AgCl was used as a “state-of-the-art” –reference although it is not possible for implantation due to AgCl-layer’s toxicity and solubility. All the materials were available in two sizes, the other being half of that of the first one. The impedance was measured by using a new, simple method to determine the impedance of the electrodes which utilizes square wave generator and data acquisition card. To obtain the result, the inter-electrode resistance has to be known or estimated somehow. In this case, it was estimated based on a finite element method (FEM) simulation and conductivity measurement of the electrolyte. The results of the electrode noise measurements are shown in Fig. 2.4.1.



a. b.

Figure 2.4.1. Comparison of the rms-noise levels between three different electrode materials in different electrolytes (PBS, NaCl and SBF) for two sizes (figures a and b).

Several different electrolytes were used in this research as well. Simulated body fluid (SBF) and phosphate buffered saline (PBS) were used together with saline. SBF is the most complex solution of these three mimicking to some extent the environment in the body. SBF takes the bone contribution into account and has a temperature dependent pH which led to measurement container that can be warmed up. Typically the measurements are conducted in saline but we wanted to examine the differences in the electrochemical properties of electrodes in different electrolytes. It was interesting to notice that the electrolyte does account to the measurement result although the differences in the conductivities of electrolytes are somewhat small. Therefore it is suggested that measurements concerning the electrochemical properties of electrode materials should be done in a solution that lies as close to the actual application environment as possible.

The corrosion durability of the electrode materials (Pt, Au and SS) was tested in a controlled environment chamber at temperature of +37 °C. The electrodes were placed into PBS and NaCl solutions and a four-week-period of investigation was run through. The electrodes were photographed once a week to see the propagation of a possible corrosion. A scientific article was written based on this research and sent to IEEE Transactions in Bioengineering but it was rejected due to lack of statistical measurement data. The article was divided into two parts. First of them dealt with the impedance properties of different materials in different materials. The article was presented in IEEE EMBC'06 conference in New York, USA, August-September 2006. The second article deals with the electrochemical noise properties, and it is accepted to

Body Sensor Networks symposium (BSN2007) to be held in Aachen, Germany in March 2007.

An extensive research was made on the standardization and legal part of the design process of an implantable device in summer 2004. ISO 9001, ISO 13485 and FDA Design Control Guidance were revised and a summary of those was written. Action aims at helping the work of the research group in determining how to do the research and documentation. Complete understanding and obeying of these guidelines allow also the resulting devices to be brought fairly simple to the market since the authorization requirements have been fulfilled.

A Master of Science thesis was made in the Institute that deals with passive resonance sensors [29]. In the thesis several different passive sensors were being designed and tested in laboratory. The passive resonance sensors are sensors that rely on a coupling between an external reader device and the sensor.

The sensor is basically a LCR-resonance circuit and the connection between the reader and the sensor is a transducer. When the secondary circuit (LCR) is in resonance with the primary circuit, the impedance of the primary circuit virtually decreases. By keeping two of the components in the secondary circuit fixed, one can calculate the third when the resonance frequency of the circuit is known.

Several prototypes were constructed and passive resonance circuits were tested in three different cases: First, a stent sensor was prototyped. A stent sensor would indicate whether the stent has opened correctly or not. However, it became clear that the opening of a stent with small diameter is difficult to measure. The sensor would be more like an on/off –sensor that indicates if the stent has not opened at all, or that it opened correctly. Basic problem in this application was the extremely weak coupling between the primary and secondary coils.

The second prototype was a resistive resonant sensor simulating a strain sensor. In a strain gauge the resistance of the sensor alters with altering strain. This contributes to the half width of the resonance curve. By measuring the width of the resonance, one can calculate the value of the resistance, hence the strain is obtained. Measuring the half width of the resonance curve is more difficult than measuring the frequency of the resonance, and therefore this may not be an extremely accurate sensor. However, it was proven that also this sensor worked out well as a prototype (Fig. 2.4.2).

The third prototype deals with the last possible parameter to be measured from a LCR-resonance circuit: Capacitance of a varactor (voltage controlled capacitor) was measured over the inductive transducer link. Measurement of a capacitance is interesting in situations where a miniaturized capacitive pressure sensor is being monitored. This prototype was also successful. Measurement of the capacitance was done by measuring the resonant frequency (Fig. 2.4.2).

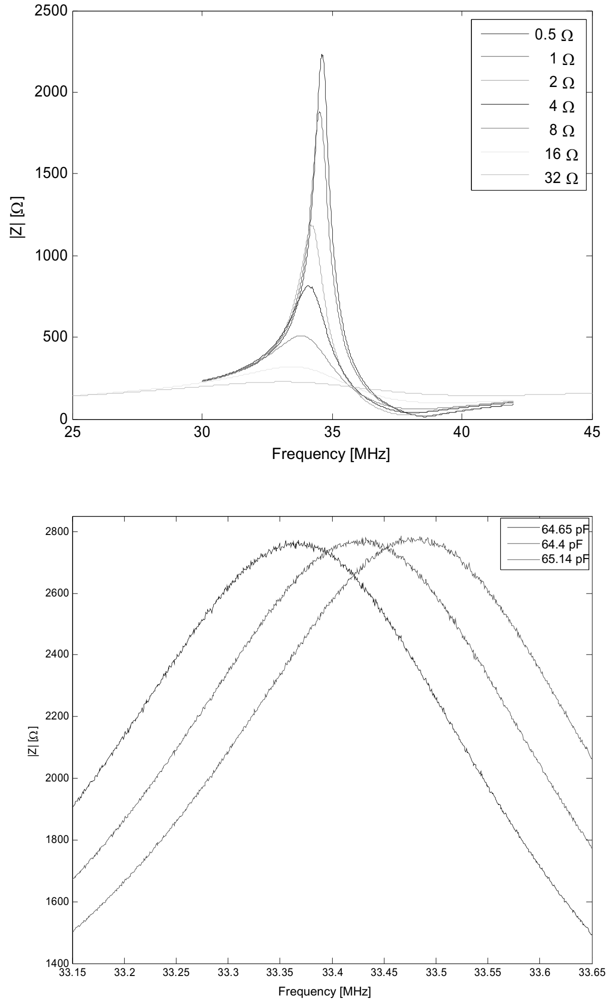


Figure 2.4.2. Impedance spectrum curves of resistive (upper curve) and capacitive (lower curve) resonant sensor prototypes.

2.4 Progress Report: Progress by the Ragnar Granit Institute

Implantable ECG devices provide a continuously available monitoring system and more stable and noiseless measurements compared to body surface ECG measurements. Modeling of physiological systems and electrical activity of human heart furnishes an effective means of studying the effects of implantation on ECG measurement prior to any clinical tests. Modeling can be applied e.g. when the location or the effects of electrode implantation and implant dimensions are studied. Especially the use of modeling in designing of implants reduces the need for expensive testing and iteration rounds in that different characteristic of the implant, such as dimensions could be tested with models thus providing the designer with crucial information. Furthermore, modeling allows estimation of signals measured from implants and the way measured signal correlates with the ECG measured from standard surface lead.

The numerical and analytical element methods, like finite difference method (FDM), have been applied when properties of human body and measurements are modeled. Mainly the FDM have been applied because it allows the implementation of complex anatomic geometries from the image data and the bioelectric fields can be calculated easily within the whole volume conductor model. We have applied realistical 3D volume conductor models of human body like presented in Fig. 2.4.1. These models serve realistical enviroment for studying the behavior of the measurements when implants are used.

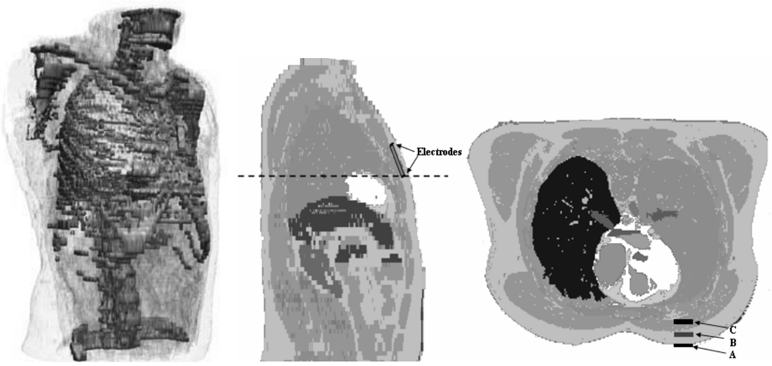


Fig. 2.4.1. 3D model of human thorax with implantable ECG monitor applied in modeling studies.

During the WIRELESS project the lead field approach together with reciprocity has been efficiently applied in studying the measurement sensitivities of the bioelectric measurements. The method is effective and applicable because the sensitivity distribution of the bioelectric measurement lead can be solved at one calculation by defining only the electrode locations instead of defining all the sources in the source volume and calculating separately the measured field generated by each source. These properties enable the fact that we can efficiently study the measurement sensitivities of various implantable monitor designs in various implantation locations in the human body. Thus there is far less need for in vivo trials during the design process. These element and modeling methods has been applied and validated in the former research projects in Ragnar Granit Institute.

We have been concentrating in modeling the measurements with implantable ECG monitor and the properties of implants. Especially the changes in ECG measurement due the implantation or implant design are concerned. We have applied FDM and lead field methods in studying the effects of implantation and implant design on the measurement sensitivities [1, 3, 6, 11, 13]. The calculations have been executed with the bioelectric field software developed in Ragnar Granit Institute. The calculation of a lead field for the 2.6 million element model took time approximately 10 to 15 minutes. Thus these methods enable efficient and inexpensive testing and reviewing of the measurements sensitivities of the implantable bioelectric measurement devices. The results of these studies indicated that implanting the measuring electrodes under the skin has minor effect on the measurement sensitivity (Fig. 2.4.2) [1, 3, 6] compared with implanting the electrodes under the costals or even on the heart muscle [1]. The effects of ECG implant dimensions [3] on measurement sensitivity have been modeled and the study showed electrode separation to be the only dimension having a major effect on measurement sensitivity. The focus of the measurement sensitivity of ECG implant has been studied [1] to predict the source region in the heart from where the measured signal arises.

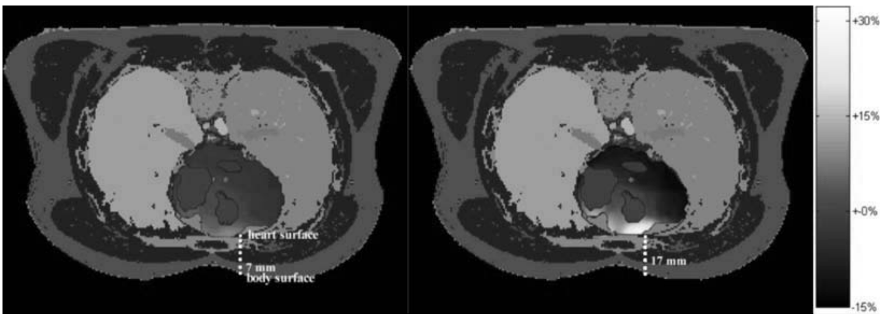


Fig. 2.4.2. Effects of 7 and 17 mm electrode implantation on the sensitivity distribution within myocardium

As part of this research a new method to analyse the sensitivity distributions of an electrode system has been developed [4, 5, 15, 18]. The new method describes the specificity of the measurement on the bioelectrical source in the region of interest in the volume conductor. This method can be applied, e.g. in analysing which implant location is most suitable to monitor anterior cardiac infarction or different arrhytmias. The results of the first simulation and preliminary experiments show that the developed parameter has a strong correlation to the signal-to-noise ratio of a measurement and it could thus be applied when SNRs of bioelectric measurements are studied and evaluated [4, 5]. Until now the method has been applied in analysing the specificity of ECG implant on 12 segments of left ventricular myocardium [15] and optimizing the electrode locations for detecting anterior myocardial infarction by modeling [21].

2.5 Progress Report: Progress by the Institute of Electronics, Personal Electronics Group

2.5.1 Measurement Platform

This chapter describes the research on the general wireless measurement platform, which uses inductive power and data transmission and provides several analog measurement channels. The platform is powered by inductive coupling using the 125 kHz magnetic field. Data transmission is realized by modulating the magnetic field. The platform has up to four 10-bit analog channels. The sample rate of the platform is 237 samples per second, which is divided between the used channels as needed. With 2.85 V supply voltage the measurement platform has power consumption less than 1.5 mW. Nevertheless the end application's total power consumption depends on the measurement set-up. Except for the antenna coil, the measurement platform is made using the commercially available components. Main target application for the platform is implantable electrocardiogram (ECG) measurement. At this stage ECG measurements are done with one channel. Additional channels are available for example for other ECG channels, temperature or acceleration measurements.

Most of the existing electronic implants, such as cardiac pacemakers, are designed for controlling or augmenting the human physiological phenomena, and measurements are mostly done to adjust those controls. In addition, studies have been done to externally measure the physiological parameters of humans or animals. Some state-of-the-art work in this field is done for example by CardioMEMS. Implantable radio frequency identification (RFID) is widely used in animals and also in some human targeted applications, such as VeriChip's human-implantable RFID microchip. This report introduces a multipurpose measurement platform for implantable or other wireless short-range measurements. The platform combines the power and data transmission used in low frequency RFID and measurement of physiological or other signals of interest.

In order to reduce the size, weight and complexity of the platform, no batteries are used, but the energy is transferred wirelessly to the device. The platform receives power by means of inductive coupling using the carrier frequency of 125 kHz. The magnetic field used for power transfer is also used for transferring data to and from the platform.

The platform has four analog inputs, which can be configured to measure for example electrocardiogram, electromyogram or temperature. The power for the additional measurement circuitry can be fed from the measurement platform. Platform converts the analog signals into digital form and sends data out by modulating the magnetic field.

Platform is accompanied with hand-held, battery-powered reader device, which creates the magnetic field and handles the data communication between the platform and external processing system, such as a personal computer (PC).

Fig. 2.5.1 shows the block diagram for the platform. The platform is powered by inductive coupling formed between the antennae of the platform and reader device, which are LC resonance circuits tuned to 125 kHz. Data is transmitted by load modulation within the same magnetic field as power. The same principle is used for example in passive low frequency (e.g. 125/132 kHz and 13.56 MHz) RFID systems[5].

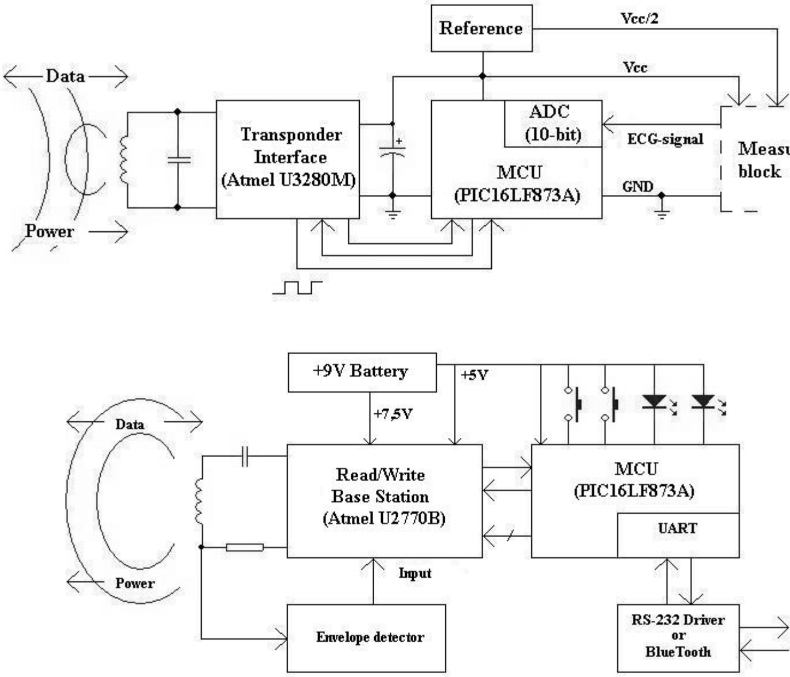


Fig. 2.5.1. Platform block diagrams. ICs used in the implementation are in parentheses.

A prototype implementation of the platform was done in order to test and demonstrate the system. Transponder interface circuit (Atmel's U3280M) is used for voltage rectification and regulation and for bi-directional data transmission. It also includes 32x16 -bit EEPROM, which could be used for additional data storage. EEPROM can be accessed through the circuit's two-wire serial communication interface. U3280M regulates the 2.9 ± 0.3 V supply voltage for the rest of the platform from antenna voltage[6]. Transponder circuit modulates the antenna voltage according to the data signal sent from the micro-controller. U3280M has also an output (NGAP) which change its state based on the state of the antenna voltage – NGAP is high when the 125 kHz carrier is present at the antenna, and low when it is not present at the antenna. Commands are sent from the reader device to the platform by switching the magnetic field off for a

[5] K. Finkenzeller: RFID Handbook – Fundamentals and Applications in Contactless Smart Cards and Identification, Second Edition, John Wiley & Sons Ltd, 2003.
[6] U3280M Transponder Interface for Microcontroller. Datasheet. Atmel Corporation 2003.

short period of time. These gaps in the magnetic field and furthermore at the platform antenna voltage is detected as negative pulses in NGAP output of the U3280M [6]. On-board capacitors provide the supply voltage during the field gaps.

The micro-controller (Microchip's PIC12F683, MCU) has an internal 4-channel, 10-bit analog to digital converter (ADC). MCU receives an analog signal from the measurement block and converts it to a digital form. Conversion result is stored as a 16-bit word, in which six most significant bits can be used for identifying the measurement and/or the device itself. Result of the ADC is coded using the differential bi-phase (DBP) coding and sent to U3280M's modulation input. U3280M's NGAP output is connected to MCU's input for receiving the commands sent by the reader device. MCU uses its internal 4 MHz oscillator for the clock source, though with the earlier prototype external 4 MHz resonator was used. There is also the in-circuit serial programming (ICSP) interface on the platform for re-programming the MCU's application code.

2.5.2 Data Transmission

Coding for data transmission from the platform to the reader device is implemented using DBP-coding. Changes at the start of every bit, as shown in Fig. 2.5.2, can be used for synchronization and error detection. Data is sent with two bytes, high byte first, most significant bit (MSB) first as shown in Fig. 2.5.3. Final sample rate was 237 samples/s, yielding the bit-rate of 3792 bit/s.

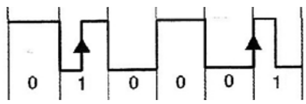


Fig. 2.5.2. DBP-coding.[5]

High Byte					Low Byte		
MSB Bit 15	...	Bit 10	Bit 9	Bit 8	Bit 7	...	LSB Bit 0
6 Reserved Bits			10 Data Bits				

Fig. 2.5.3. Data packet sent by the platform.

The sample rate is divided between the used ADC channels. Therefore sample rate per channel depends on the final application.

2.5.3 Implantable electrocardiography

One of the major applications for the measurement platform described in this paper is implantable ECG measurement. This chapter shortly describes such an application and some of its essential parameters and in vitro results.

As shown in Fig. 2.5.4, ECG amplifier block including high-pass filter at the electrode inputs, differential amplifier, and second order Sallen-Key type low-pass filter, was connected to one of the platform's analog inputs. Measurement block's supply voltage was provided by the platform. Also, the reference voltage with amplitude of half of the supply voltage was fed to the amplifier. Three electrodes, two for measuring and one for grounding, were connected to the measurement block.

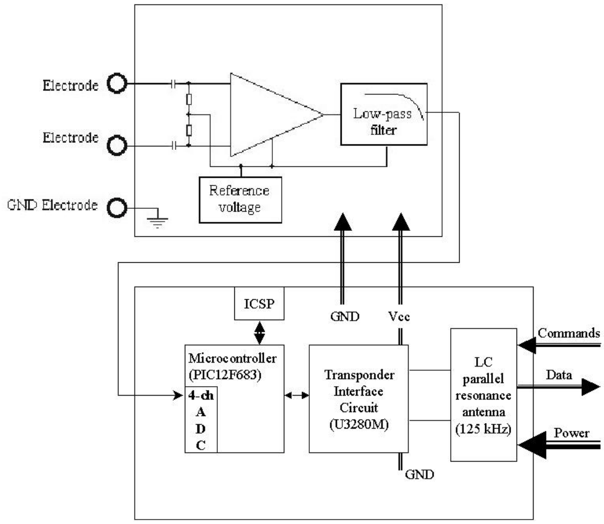


Fig. 2.5.4. ECG application block diagram.

Electrodes were placed on the chest at standard points V2, V3, and V4 used in the 12-lead ECG measurements. Resulting output is displayed in Fig. 2.5.5.

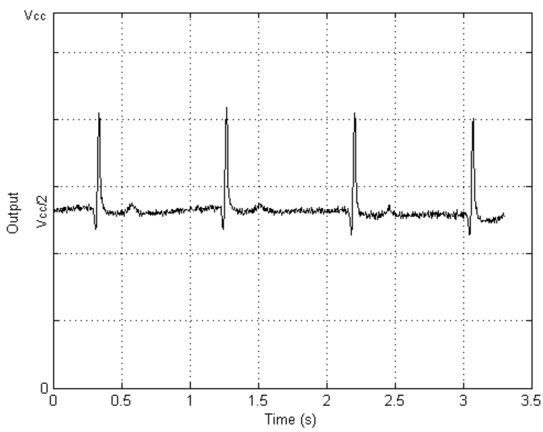


Fig. 2.5.5. Measured surface-ECG.

Photographs of the implemented electronics are in Figures 2.5.6 and 2.5.7.

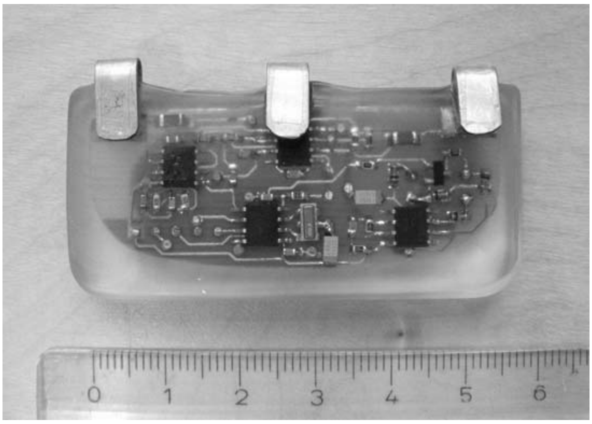


Fig. 2.5.6. The front side of the encapsulated implant showing electrodes and electronics.

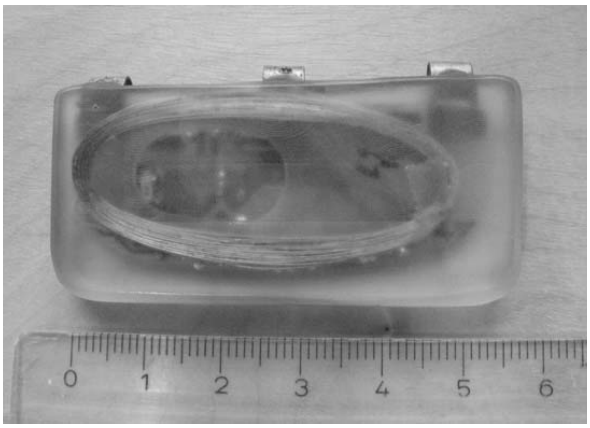


Fig. 2.5.7. The back side of the encapsulated implant showing the transmission coil.

2.5.4 Power need

Measurement platform's current consumption was measured with Fluke 87 True RMS multi-meter from U3280M's regulator output with no additional circuitry connected to analog inputs. Since the internal current consumption of U3280M itself was not measured, the total current consumption of the platform (I_{tot}) can be calculated with

$$I_{tot} = I_{CC} + I_{Fi} + I_{FC} \quad , \qquad (2.5.1)$$

where I_{CC} is the measured current consumption which equals 425 μA, I_{Fi} is U3280M's operating current during field supply which is typically 40 μA [6], and I_{FC} is U3280M's FC output's current consumption. FC-pin outputs the clock signal of 125 kHz extracted from the antenna voltage and has a current consumption typically 50 μA [6]. NGAP pin is low only when the magnetic field is not present, for example while sending commands from the reader device to the platform. Most of the time NGAP is at high state, in which its current consumption is –150 μA (U3280M sinks the current into NGAP pin)[6]. Current consumption caused by the NGAP pin is included in the measured I_{CC}. Currents are also shown in Fig. 2.5.8.

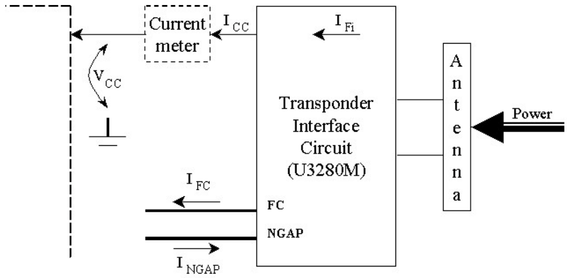


Fig. 2.5.8. Currents in the platform

Using (2.5.1) and currents mentioned above, the measurement platform's total current consumption is found to be 515 μA. Current consumption caused by the ECG measurement block was measured as 156 μA.

Platform's supply voltage is defined as the rectified and regulated voltage which U3280M's outputs at its VDD output. The voltage is characterized as 2.9 ± 0.3 V [6]. Measurements showed that the voltage varied from circuit to circuit and it was typically found to be around 2.85 V. Using the 2.85 V voltage and currents mentioned in chapter 4.1, the total power consumptions of the platform without and with the ECG measurement block were found to be approximately 1.47 mW and 1.91 mW, respectively. Table 2.5.1 lists the current and power consumptions for the platform without and with the ECG measurement block.

TABLE 2.5.1

PLATFORM'S CURRENT AND POWER (VDD = 2.85 V)

	Current	Power
Without ECG Block	515 μA	1.47 mW
With ECG Block	671 μA	1.91 mW

2.5.5 Operating Distance

Defining the minimum power consumption of the platform, or its end application, is closely related to its maximum operating distance. Hence, the lower the power need of the device, the greater its operating distance from the reader antenna. Reliable operating distances for platform and ECG application are presented in table 2.5.2.

TABLE 2.5.2

OPERATING DISTANCE

Without ECG Block	58 mm
With ECG Block	30 mm

During the data transmission, the operating distance is actually limited by the reader device's receiver sensitivity. While distance is grown, errors in data transmission are detected before the platform looses power. Therefore, in a case of ECG application, the maximum operating distance was defined as the distance in which the data transmission is still reliable.

2.5.6 Future development of the electronics in the measurement platform

The multi-channel measurement platform intended for small-sized, low-power wireless measurements, such as implantable electrocardiogram, has been developed. Platform has total of 4 analog inputs channels and can provide a supply voltage of 2.85 V to the measurement block attached to it. Power was transferred with inductive coupling at 125 kHz. Data transmission was realized by the means of load-modulation, widely used in low-frequency RFID applications. With the sample rate of 237 samples per second surface-ECG was measured, sent to the hand-held reader device and furthermore displayed in the computer screen.

In the electronics point-of-view, some of the main concerns are the physical size of the platform, higher data rate, and low power consumption. In addition to the platform's power consumption, some of the main issues concerning the operating distance are magnetic field carrier frequency, dimensions and inductances of the antenna coils, and power available for the antenna driver of the portable, battery-operated reader device. Work for using the higher carrier frequencies and also multiple measurement platforms in the vicinity of one reader are now ongoing. Also, miniaturization of the platform and in-vivo measurements with the ECG-prototype coated with biocompatible coating will be done.

2.5.7 Alternative power and data transfer methods

The research on wireless power transfer into an implantable device has developed further in the direction of alternative methods. In addition to the inductive power transfer used in the implementation of the implant architecture, acoustic power transfer has also been investigated.

Wireless implantable devices have a huge potential in the field of biomedical engineering. One hard problem to be solved is developing a satisfactory power supply. We have done research on a novel ultrasound-based method for powering a battery-free electrical implant. Contrary to the commonly used RF and inductive methods, ultrasonic power transmission helps to avoid problems with electromagnetic coupling and offers a selection of data frequencies not limited by national regulations. The proof-of-concept equipment is based on piezoelectric crystals utilized to both transmit and receive ultrasound. *In vitro* measurements in degassed water were carried out to bring perspective to the pros and cons of the ultrasonic link. A 63 % of maximum power efficiency at the distance of 12 cm was achieved.

Research of acoustic energy and data transmission in implantable applications

In implantable applications, tissue compatibility, safe energy levels and long-term durability play an important role. State-of-the-art implants and implant prototypes use electromagnetic-based communication and energy transfer methods despite of the fact that the field of the most commonly used antennas is attenuated quite efficiently along the distance. The field is also prone to disturbance caused by external magnetic fields, or it may interact with them in an unwanted way.

The feasibility of ultrasound-based power and data transmission for implantable applications has been studied in co-operation with the Medical ultrasound research group of the University of Kuopio. The power transmission link consisted of two piezoelectric wafers that were utilized with a 840 kHz frequency. The transmitter and the receiver were run in degassed water, and the impacts of different distances, angles, media and loads on the transmission efficiency were studied. The transmitted power varied between 250 mW and 1 W. Test measurements with a focusing transmitter were also carried out. Tissues with different thicknesses were modelled with polyvinyl-acrylic (PVA-C) phantoms prepared for the purpose, and special emphasis was put to matching impedances between the crystal and the load while designing the circuit. Figure 2.5.9 shows the circuits used for power generation and reception.

All measurements were carried out in a bowl of degassed water. The efficiency varied between 21 and 35 % at distances between 5 mm and 105 mm. The distance did not affect the transferred power significantly, but a standing wave was generated between the transducers causing strong variation in both received and transmitted power. The standing wave maxima and minima occurred every half wavelength and the power levels varied ± 60% from the mean value. The tissue phantoms did not affect the transmission significantly, but turning the receiver with respect to the transmitter caused a rapid drop in the received power already at angles of a few degrees. The same happened when the receiver was moved sideways across the transmitter. Figure 2.5.10

shows the results obtained in distances of 5 - 105 mm and Fig. 2.5.11 the results when the receiver was turned or moved with respect to the transmitter. The forwarded power was kept at 250 mW during the transmission.

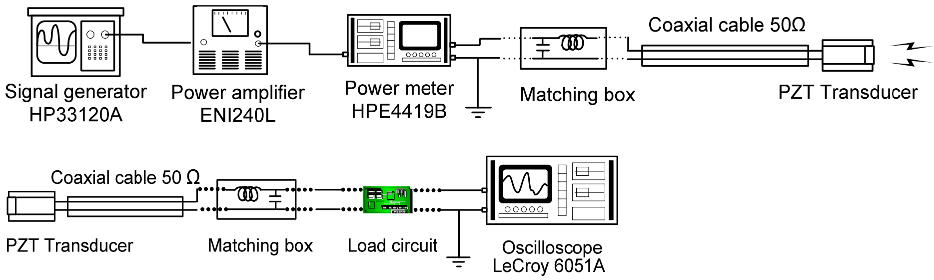


Figure 2.5.9. Top: power amplification circuit. Bottom: power reception circuit.

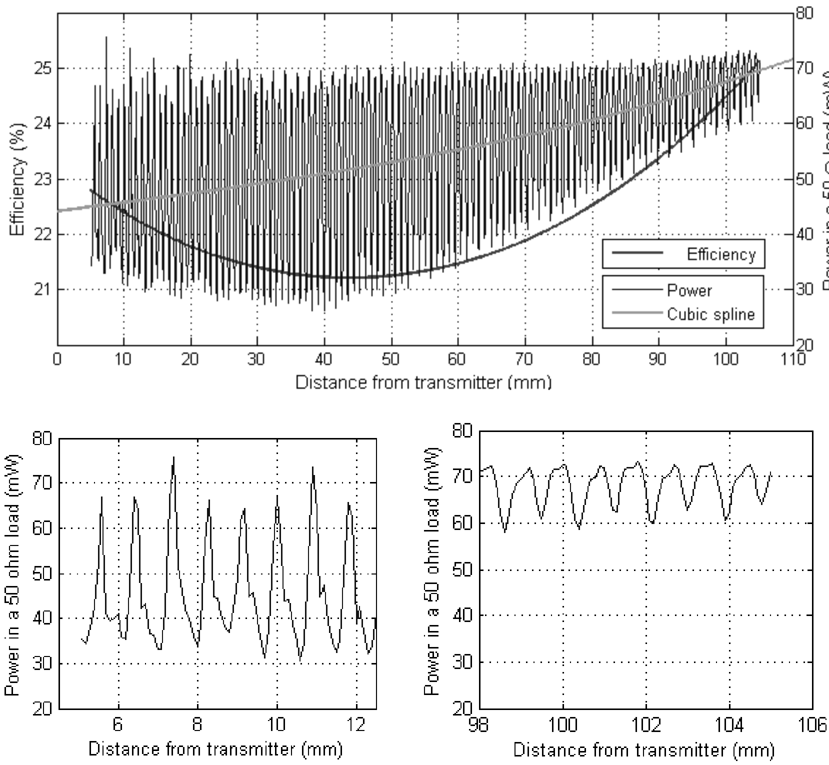


Figure 2.5.10. Total efficiency and received power as a function of distance between the transmitter and the receiver. The cubic spline curve represents the average of the received power. Bottom left: magnification of the received power close to the transmitter. Bottom right: 98 - 105 mm distance from the transmitter.

The possibility of data transmission was tested by changing the load in the receiving circuit and detecting changes in the transmitting side. Short-circuiting the receiver or using a very small load resistance caused a significant drop in the transmitted voltage. Thus it can be deduced that it is possible to modulate data to an acoustic field in the same way than in inductive applications.

The results indicate that ultrasound can be used to transfer power, and data transmission by load modulation is also possible. The transducers must be kept in place during the transmission to provide stable and sufficient flow of power to the implanted device.

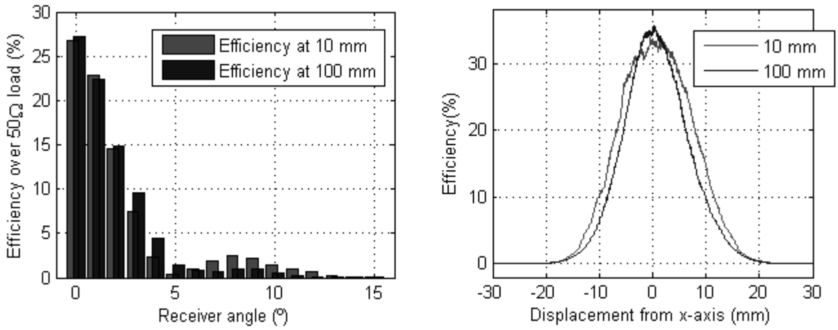


Figure 2.5.11. Left: Turning the receiver with respect to the transmitter. Right: moving the transmitter across the receiver.

The efficiency, range and transmitted power levels are, with certain restrictions, better than in electromagnetic methods. The unlimited frequency range in data transmission compared to electromagnetic-based methods, for which the law allows only specific frequency bands, and usability in environments sensitive to electromagnetic fields make the acoustic power and data transmission an option to be reckoned with.

Photographs of the measurement equipment and the transducers used in the power transfer measurements are in Figures 2.5.12 and 2.5.13.

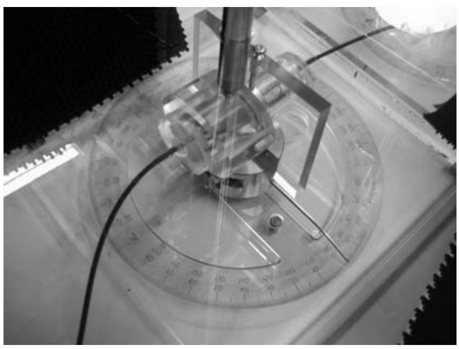


Fig. 2.5.12. Measurement system for the radiation beam shape showing the transmitting and receiving transducers together with the turntable.

Fig. 2.5.13. Ultrasonic transducers used in the power transfer measurements.

2.6 Progress Report: Progress by the Institute of Electronics, Packing Group

Aim of this project to microelectronics packaging group is to study different packaging technologies in implantable devices. It is important that the device is reliable, small and lightweight. To achieve this, different new packaging techniques can be used. Direct chip attachment (DCA) saves space on circuit board and reduces weight. Flexible circuit boards are thinner and lighter and they can be rolled or folded up to a shape wanted. 3D packaging enables the use of z-axis in packaging of electronics. With 3D structures the packaging efficiency can be up to 300 - 400%. This saves space tremendously.

In this study different packaging techniques suitable for implantable devices have been studied together with the effect of different coatings and sterilization means. Since the device needs maximum miniaturisation, flip chip technique has been the main technology studied. In flip chip technique the pure silicon chip is attached to circuit board active side facing down. Connections are formed through conductive bumps that are formed on the I/O –pads of the chip. Either solders or conductive adhesives can be used to form the connections. Since solders have lead and other hazardous substances, we have studied conductive adhesives. Joining has been done using anisotropically conductive adhesive, which only conduct in z-direction. Figure 2.6.1 shows flip chip component with anisotropically conductive adhesive. Polymer materials tend to absorb water and that is one reliability issue with conductive adhesives that needs to be studied.

Component used in reliability testing were 8mm x 8mm flip chip components. The basic FR-4 was used as substrate material and anisotropically conductive adhesive (ACA) was used to interconnect the chips on substrates. Six different test lots with different coating and strilization methods were done for reliability tests. Reliability testing of the samples

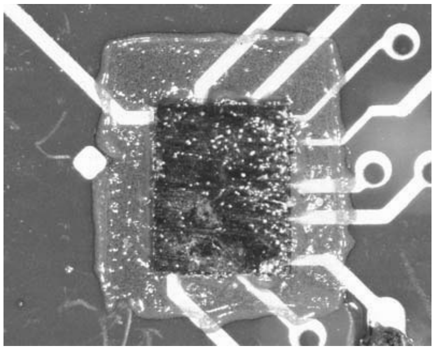


Fig. 2.6.1. Flip chip component joint with anisotropically conductive adhesive.

is done in temperature-humidity chamber, and the samples can be tested real time during the tests. Reliability testing has been done according to standard JESD22-A101-B, where temperature is 85 °C and relative humidity 85%. One test lasts 1000 hours. Aim of this test was to show the reliability of electronics in humid environment. Test chips have test structure where the daisy chain resistance of the chip can be measured. The interconnections can be monitored and when one interconnection fails it can be seen from the daisy chain resistance. Figure 2.6.2 shows an example of the measurement data from measuring the daisy chain resistance. The voltage across the conductive bumps is measured and can be seen from the figure. As can be seen the sample is not working in room temperature but it is working in 85/85 –conditions.

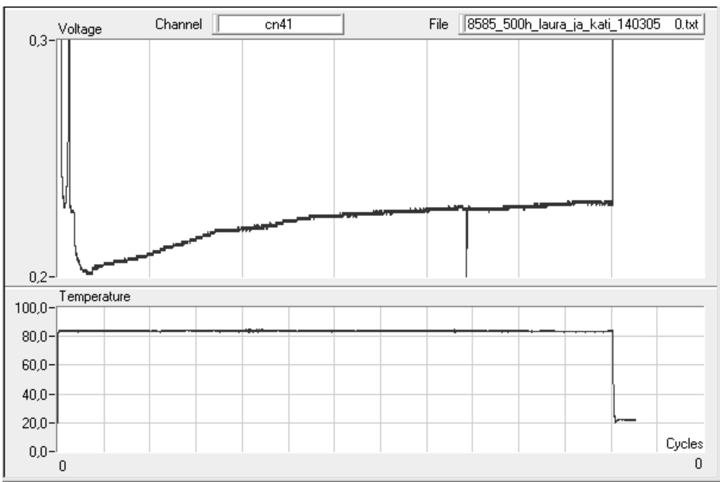


Fig. 2.6.2. Measurement data from humidity testing. This sample is conducting in 85°C but is not working at room temperature.

The low-power issues were studied in the last project year. It was soon realized, that the data-modulation scheme used in the first prototype versions dissipated much power.

Different data-modulations were tested to get lower power consumption and better data-modulation. Normal resistive load-modulation was used as reference. An inductive load – working same time as a part of the power source – enables good power supply and long read distance (Fig. 2.6.3), as energy is stored in a magnetic field instead of being dissipated by a resistive load. Commercial data transfer circuit (resistive load modulation) was left out from the second prototype version.

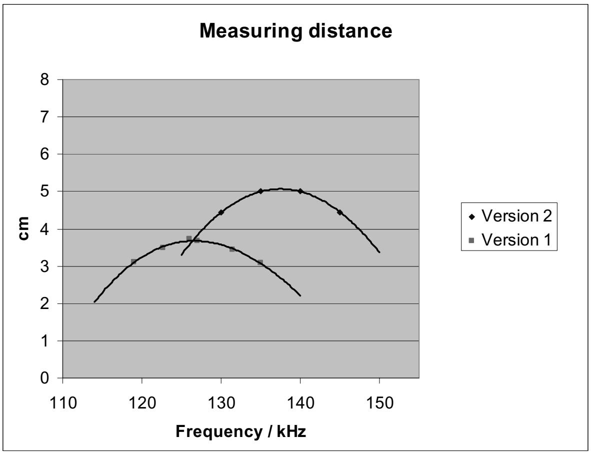


Fig. 2.6.3. Read distance with a constant supply voltage.

For miniaturization, all components for the second prototype were selected so that their package is very small (Fig. 2.6.4). As the low-power issues were considered the most important topic in the third project year, miniaturization could not be done. However, the components are selected so that miniaturization of electronics should be a relatively easy task. Most problematic issue for miniaturization seems to be the coil used for inductive data and power transfer.

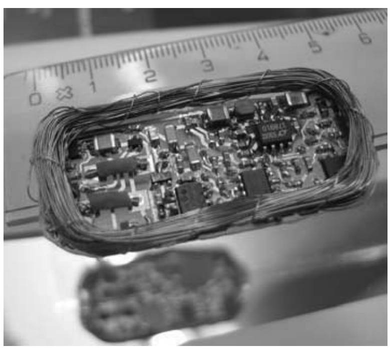


Fig. 2.6.4. Implant with new data-modulation and temperature measurement.

The second prototype included also a temperature sensor, since the body temperature is an important parameter for many physiological systems. This was implemented using NTC thermistors as sensors. Therefore, it is important that the power supply voltage is constant. In addition, resistivity of the coating of the device should be insensitive to e.g. moisture, as the sensor is implanted. Parallel resistance with sensors could affect the measurements.

Electrodes have to be in direct contact to tissue to have proper signal. Therefore, the electrodes should be made of biocompatible metal, e.g. gold. Soldering of gold electrodes was problematic, since the liquid tin easily wetted the electrodes, and tin is not biocompatible. In addition, inter-metallic layers of tin-gold were formed. Therefore, the electrodes were mounted with conducting adhesive (Fig. 2.6.5). The sensor was finalized with a parylene coating that was removed from the electrodes; thus, the only materials on the surface of the implant were gold and parylene.

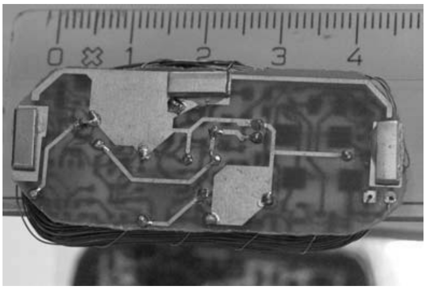


Fig.2.6.5. Three gold electrodes fasten with conducting adhesive.

The surface of the implant should be planar and should not have any sharp edges for easy implantation. In the second prototype, the electrodes were on the same surface as the epoxy coating, as depicted in Fig. 2.6.6. The excess epoxy was mechanically grinded from the sensor such that the gold electrodes were uncovered. In this was, an easily implantable sensor and electrode shape was achieved.

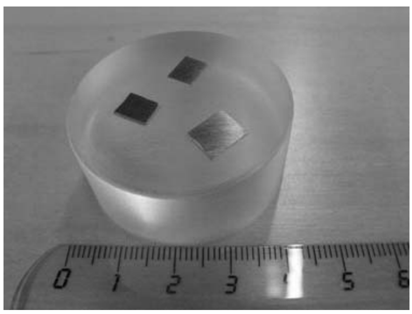


Fig.2.6.6. Electrode configuration.

Other issues briefly studied were the reader antenna and real time thickness measurement of parylene coating.

2.7 Progress Report: Progress by the Institute of Biomaterials

Implantable wireless electrical device will be exposed inside the human body to the highly corrosive and aggressive electrolytic medium in the mechanically stressful conditions. This causes excessive demands for coating materials. The used materials have to be biocompatible and form stable structure in order to enhance desirable tissue reactions and to prevent unwanted tissue reactions, such as fibrous tissue capsule formation, inflammation reactions or even necrosis. The coating should not be penetrated by the body fluid, the particles and molecules of materials and surrounding tissue, which may react chemically resulting in corrosion products release to the tissue interface, and cause the short-circuiting of the passive components or the failure of the active components. Therefore, the electrical device has to be sealed hermetically with uniform coating without pinholes. The surface of the implant has to be modified shaped suitable for assigned anatomical site and it must not contain corners and edges that could cause pressure damage of the adjacent tissue. In addition, the coating material has to have suitable dielectric properties and to maintain its electrical and mechanical properties during its expected lifetime. It also has to resist sterilisation process. The excellent protection for electronics is achieved continuous coating, which have low water absorption, and which does not degrade or loose adhesion to its substrate even in the long-term exposure. In order to minimize the injury of tissues in the surrounding of device, the device should to be anatomically shaped and small-size. Flexible and anatomically shaped device can be achieved using polymeric materials (such as silicone and epoxy), and therefore during this project it has mainly been concentrated on polymers as an encapsulating material. However, the challenge of polymers is their water permeability that may inhibit the achieving of fully hermetic structure, and therefore their permeability properties has to be tested carefully. All these factors has to be considered in Institute of Biomaterials, when coating materials are selected, processed and tested for implantable electrical devices.

In Institute of Biomaterials the tasks have been the selection, processing and testing of coating material, especially polymers for the enclosure of implantable sensor and measuring system. Besides above mentioned factors, the curing conditions, such as curing temperature and time are also important factors in the selection of materials. Based on material comparison three polymers (silicone, epoxy and parylene C) and coating methods (dip coating, spray coating, cast moulding, vapour deposition polymerisation) have been selected for further study. Two of those coating methods were found applicable: mould casting (silicone and epoxy) and vapour deposition (parylene C). The selected medical grade materials are biocompatible, stable and well-known materials, which have been used in the medical applications. The testing methods of coating materials have been developed in order to study their absorption, permeability and adhesion, and the properties of selected materials, and also the coating methods have been studied in two Master of Science thesis.

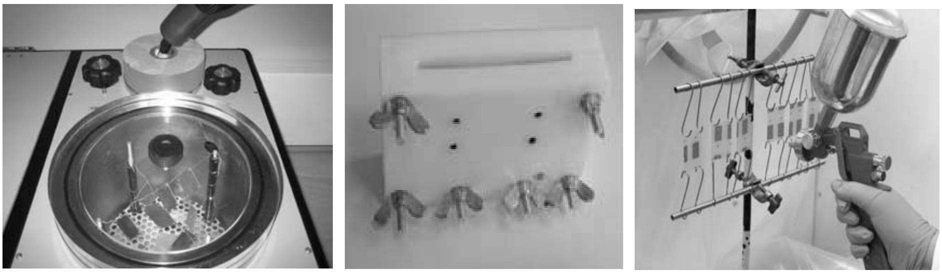
Results

Three applicable medical grade coating materials were selected and tested. Selected silicone is a platinum-cure two-part PDMS (polydimethylsiloxane) silicone elastomer dispersed in xylene (MED-6640 Silicone, NuSil Technology). It cures at 100 ^{o}C in four hours. Epoxy is a diglycidyl ether of bisphenol A epoxy with a polyoxypropylene-diamine hardener (Epo-Tek 301-2FL, Epoxy Technology, Inc.), which cures at room temperature in three days. Third studied coating material is poly-para-xylylene C (Galxyl C, Montell), which has commercial name Parylene C. Parylene C coating is applied to substrate by vapour deposition polymerisation (VDP) at room temperature (Para Tech Coating Scandinavia Ab, Järfalla, Sweden). In order to combine the material properties of these three polymers it has been also studied the composite layer by layer structures of the polymers. These materials were used as coatings for FR-4 circuit boards, test chips and ECG-prototypes.

Coating methods

Different coating processes have been studied: dip coating, spray coating, mould casting and vapour deposition. Dip coating system consisted of a dip tank, made of Teflon, and a drive mechanism (a Lloyd LR 30K materials testing machine, Lloyd Instruments Ltd, Fareham, England) (Fig 2.7.1). The device was automatically dipped into a tank containing the liquid coatings. After immersion, a device was withdrawn at a controlled rate and cured. In spray coating method (Fig 2.7.2.c), the fluid was sprayed as fine droplets to the surface of device and then cured. The thicker coating layer was achieved by cast moulding. In this method the device was placed to the specific casting mould and the polymer was poured to the mould. Two types of moulds were used, a sink and two part shell moulds. After curing the test sample was removed from the casting mould. The used moulds were made of Teflon (Fig 2.7.2.b) or silicone. In vapor deposition method the powdered parylene precursor, dimer is vaporized under vacuum

Fig. 2.7.1. Materials testing machine LR 30K for automatic dip coating.



a. b. c.

Fig. 2.7.2. a. Parylene coating system, b. Mould casting, c. Spray coating.

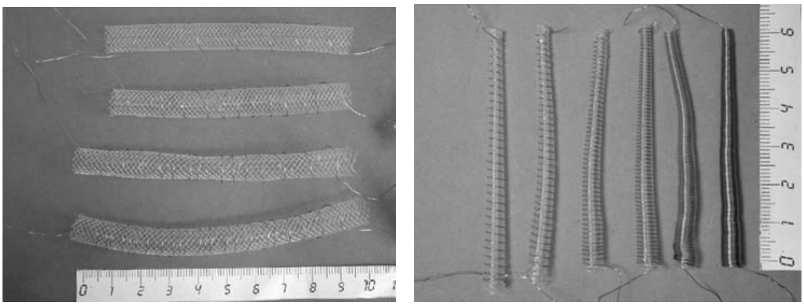
and heated to a dimeric gas (Fig 2.7.2.a). The gas is then pyrolized to its monomeric form. In room temperature deposition chamber, the monomer gas deposits to the substrate and polymerised to a layer of parylene. The process parameters for vapour deposition have been optimized and also operating and service manuals were made during study. The parameters for each coating method were optimized in the studies.

Test chips were coating by dip coating, spray coating and vapour deposition. Dip coating and spray coating methods were used with silicone and epoxy. Parylene C coating was processed by vapour deposition.

Various electronic composites and electrode materials were coated by mould casting and vapour deposition. ECG-device prototypes were also coated with composite structure of epoxy and parylene C. The devices were first coated with epoxy in Teflon or silicone mould. Parylene C layer was produced over the epoxy layer by vapour deposition.

Stent design

A simple sensor system integrated as a part of the stent was also studied. Using sensors, the opening of the stents, critical parameter for clinical function of the stent were planned to be studied. Copper wires with three different diameters and different helix angle were weaved around a complete stent structure (Fig 2.7.3.a). The nylon stents with 4-10 mm diameters were used. Helical horn-shaped spiral stents were also produced from copper wire itself and with polylactic-glycolic acid (PLGA) fibre (Fig 2.7.3.b). The function of the sensoring studies was performed by the Institute of Measurement and Information Technology.



a. b.

Fig. 2.7.3. a.Copper wires with different helix angle in complete stent structure, b. Horn-shaped spiral stents.

Device test protocols and results

In material testing the curing conditions, such as temperature and times, of silicone and epoxy were optimized by differential scanning calorimetry (DSC). *In vitro* testing was done both the coating materials and manufactured prototypes, and also to test chips. *In vitro* simulation the absorption properties of polymers in water and natrium phosphate buffered saline at 37^{o}C were measured using membranes made from studied silicone and epoxy. Tests are based on standardized test methods EN ISO 62:1999 and ASTM D570-98. Hydrolysis modified some material properties. Silicone membranes become sticky while epoxy membranes went first soft and opaque and later those went hard and bright again. Water absorption was approximately 0.5 % with silicone membranes whereas with epoxy it was approximately 3,5 %.

Effect on sterilization in hydrolysis conditions were also study. Polymer films and test chips were sterilized by gamma irradiation with ^{60}CO gun as a source of irradiation. Gamma irradiation broke electronic components therefore ethylene oxidation sterilization (+42ºC) was used with ECG-prototypes. The function of these prototypes has been tested *in vitro* at the Institute of Measurement and Information Technology. Ethylene oxidation sterilization seemed to be applicable method to electronic device, because it caused any problems in function of the electrical devices.

The permeability properties of silicone and epoxy were tested from the membranes made by mould casting process. Half of the samples were also sterilized using earlier mentioned method. Water vapor permeability of polymer is tested in humidity cabinet according to standard ASTM D2247-02, where temperature is 37 °C and relative humidity 95 %. One test lasts 24 hours (Fig 2.7.4.). Water permeability of polymer membranes was tested at 37^{o}C during 24 hours in the heating chamber (ASTM D870-97). The result of water vapor permeability and water permeability were almost same both silicone and epoxy. Silicones permeability was about 0.12-0.14 %, and epoxies about 0.01-0.02 %.

Fig. 2.7.4. Humidity and heating chamber for the permeability tests.

For adhesion testing the FR-4 laminate and FR-4 laminate with NiAu coating were covered with silicone and epoxy using spray and dip coatings. Also the composite structures were studied. Adhesion of parylene coating was tested as well. The adhesion of polymer to the substrate were tested using two test methods; cross hatch adhesion method (ASTM D3359-97) and pull-off adhesion test using Lloyd testing machine (SFS-EN ISO 4624:2003) (Fig. 2.7.5). As a summary of adhesion tests results it can be found out that epoxy has better adhesion to pure FR-4 laminate than silicone or Parylene has. To NiAu coated laminate is more difficult to have tight adhesion than pure laminate. Higher adhesion is able to achieve by dip coating technique. However, the adhesion of the coating seemed to be enough for the implantable device, which has been developed in this study.

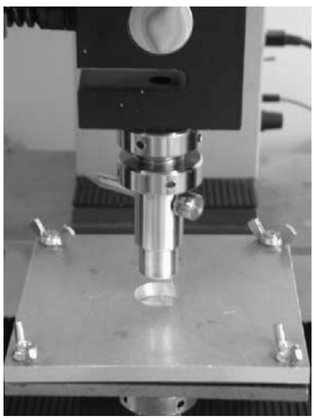


Fig. 2.7.5. Pull-off test arragements with Lloyd.

Surface modifications

Foreign body reactions and excessive fibrous tissue capsule formation to the surround of implant may interfere with the detection and function of sensing device. The growth of surrounding tissue straight on the surface of device can be enhanced, for example, by treating the surface of the device by chemically or incorporating the biomimetic structure on the surface of device. In addition, unwanted tissue reactions can be decreased by adding coating layer, which releases controllably bioactive materials, such as antibiotics. The literature review about different methods to modify surface properties has also done in Institute of Biomaterials, but it has not been possible to apply to studied devices.

Electrically conductive biomaterial

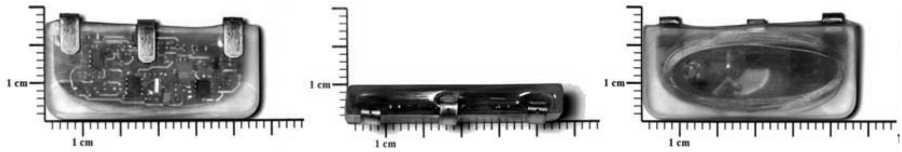
Literature review of conductive biomaterials has been done. The interest was to find electrically conductive polymer that is applicable to coat medical device or to function as a sensor by definition. The desired properties of electrically conductive polymer were non-toxic, biocompatibility, ease to process and possibly biodegradable.

Conclusions

Biomaterial know-how could be utilized in devices design. Three polymeric materials were chosen according to the pre-set requirements and were selected to coating materials for medical application: silicone (MED-6640), epoxy (Epo-Tek 301-2FL), and parylene C (Galxyl C). Two feasible coating methods found out: mould casting and vapour deposition. ECG-prototypes were managed to coat with composite structure. The device was coated with epoxy by mould casting. Parylene C coating was processed on top of epoxy by vapour deposition. Different sterilization methods effect on coating materials and electronic components could be studied. *In vitro* experiments in buffered solution were done for coating materials, test chips, and ECG-prototypes. Epoxy and Parylene C seemed to be appropriate enclosure materials to implantable electronic device. In addition *in vivo* experiments managed to do with cows. *In vivo* results are reported elsewhere in this report.

2.8. Prototypes of an Implantable ECG Monitoring System

Several prototypes of the implantable ECG-monitoring device were made. Different coils were tested to be used as receiving/transmitting antennas in the implant. It was found that a planar antenna with as large area as possible was the best alternative for powering the device. The physical form of the implant was not clear until the first *in vivo* tests became topical. The veterinarians that were responsible for the implantation of the device into cow suggested that electrodes should be as smooth as possible. In the first prototype, stainless steel (SS) was selected to be the electrode material. The electrodes were placed so that the measuring electrodes were at the ends of the device and the grounding electrode was located in the middle. The electrodes were soldered on the circuit board, then the device was coated and the electrodes were turned with pliers so that the electrodes were as much along the surface of the device package as possible. The first prototype of the implantable ECG device is shown in Fig. 2.8.1. See also the figures 2.5.6 and 2.5.7. The whole measurement system with external reader unit and coil antenna is presented in Fig. 2.8.2.

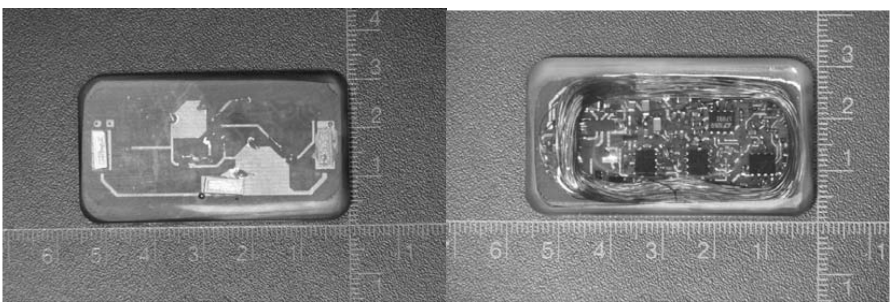


a. b. c.

Fig. 2.8.1. Structure of the encapsulated first prototype device. a. Top view, b. side view, and c. back view of the device.

Fig. 2.8.2. Inductive reader unit for the first prototype. The coil antenna is constructed inside a plastic tube in a handle.

The second prototype was a little more sophisticated device when compared to the first one. This prototype had in addition to the ECG-measurement an integrated temperature measurement. The electrode material was also changed to gold, and the electrodes were glued at the bottom of the device circuit board with conductive glue. After the coating the electrodes were polished up with an abrasive paper. The second prototype of the implant is presented in Fig. 2.8.3. See also the figures 2.6.4 and 2.6.5.



a. b.

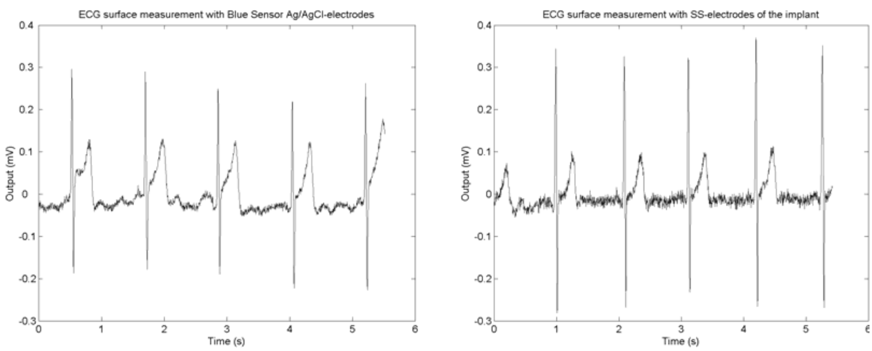
Fig. 2.8.3. Encapsulated second prototype. a. Three gold electrode plates glued on the back-side of the circuit board. b. Component side of the device with an antenna coil.

Testing the Prototype with Body Surface measurements

The performance of the first ECG-prototype implant was tested with surface measurements of human ECG (Fig. 2.8.4). Two different electrode materials, commercial Ag/AgCl and SS electrodes on the implant were used in the measurements. The commercial electrodes were attached on the prepared skin and connected with wires to the implant to get electrical connection. [56]

Figure 2.8.4. Testing of the operation of the first implant by recording surface ECG. The implant electrodes are pressed against skin.

As can be seen in Fig. 2.8.5 the signal quality with both electrodes is adequate. With SS electrodes the noise level, however, is a little bit higher.



a) b)

Figure 2.8.5. Signals measured with (a) commercial body surface Ag/AgCl electrodes attached, and (b) with implant's electrodes attached on the skin.

Testing the prototype in vivo in cows

In vivo experiments were conducted by implanting the first prototypes (Fig 2.8.1) into cows. The experiment was conducted under the licence of MTT Agrifood Research Finland, animal experiments committee, approved animal experiment, 34/2005, 16.6.2005.

Four devices were implanted for 24 hours into four Finnish Ayrshire cows. The cows were moved from the loose housing system into cubicles for surgical implantation. Each cow handled one by one, sedation, and pain relief was provided by veterinarian. A 55-85 mm incision was cut on the down of the cows left side. The implant was inserted into a subdermal pocket. Three sterile sutures were applied to secure the implantation. Implant was inserted to four different orientations to test the best possible orientation for obtaining the signal. Implant placement and different orientations are presented in Figure 2.8.6.

In this experiment only one external reader device was applied and it was kept near the cow's side during the measurement. ECG of each cow was measured in cycle of 10-20 minutes during 24 hours i.e. ECG data was recorded throughout 4 to 6 hours in total per cow. [46, 57]

Examples of cows ECG measured with implant are presented in Figure 2.8.7. It is observed that the main cardiac activity (R-peaks) are clear and thus this data could be applied when the heart rate of the cows are studied. The heart rate variability is on parameter which will be studied by Agrifood research group and the developed implant will be in important role at that research. [57]

In the experiments the external reader device was held near the cows' side by hand which caused noise and instability to the measurement. Thus the system and especially reader device should be enhanced to make it more applicable. All the measurements, especially the *in vivo* experiments, served extremely valuable information and experience which will be adopted when the implant is further developed in the future projects.

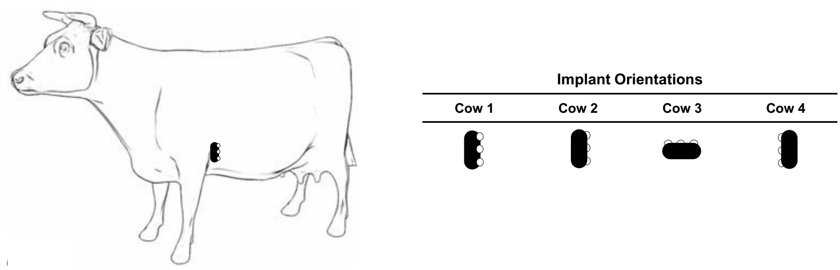


Figure 2.8.6. (A) Placement of the implant in cows. (B) Orientations of the implants. Electrodes which are presented in white were outwards in the cow 1 and inwards in all other cows. Antenna coil is always located on the opposite side than the electrodes. [56, 57]

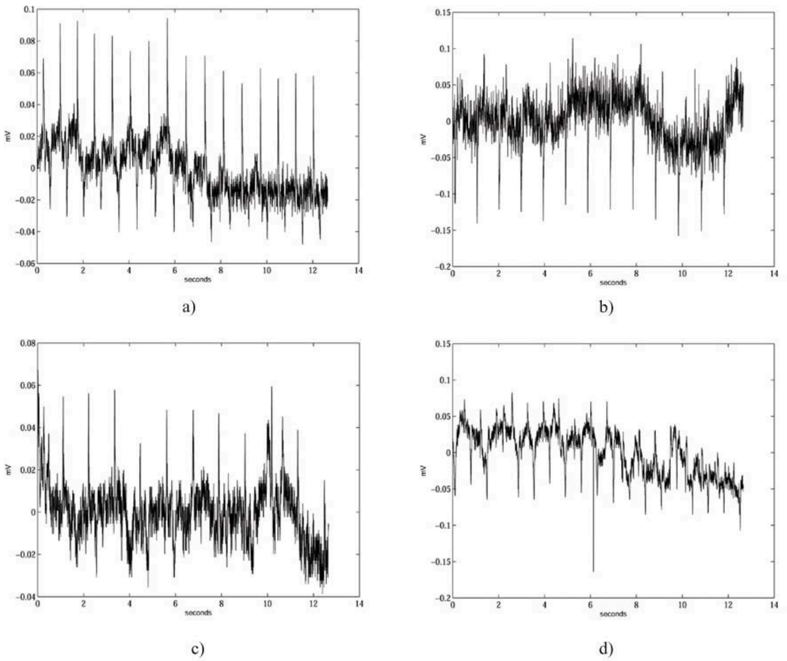


Figure 2.8.7. Example signals measured from 4 cows. The figures a, b, c and d show signals measured from cows 1, 2, 3 and 4, respectively.

3 International Aspects

After the EMBC'04 conference in San Francisco in September 2004 we visited the University of California, Berkeley Campus. Prof. Luke Lee from the Berkeley Sensor & Actuator Center presented his research on BioPOEMS and BioMEMS for advanced biomolecular chips and clinical applications. Program Manager Riku Mäkelä from TEKES, San Jose California Office, organized a serie of meetings with Dr. Mike Eklund (Postdoctoral Researcher, EECS/UC), and Shankar Sastry and Ruzena Bajcsy of the UC Berkeley-based Center for Information Technology Research in the Interest of Society (CITRIS).

As a result of these contacts an international collaboration between the group at University of Tampere, Aarhus University and UC Berkeley has been formed under an Innovation Alliance initiative. The Innovation Alliance has taken an initiative on technology creation based on user needs. Innovation Alliance aim is to create a public/private partnership anchored in Denmark, Finland and California (Fig. 3.1). The three universities form consortium for a project "Information Technology For Assisted Living At Home" (ITALH). ITALH project is aimed at increasing quality of life with a focus on the home, e.g. through better support for elderly citizens who want to stay in their own homes without forgetting the support of emerging mobile lifestyle. Even though the aim is focused to our growing senior citizen group, the project utilizes basic design for all concepts and provides general solutions for the usability and applications of new technology for home and health. The ITALH technological and service platform will include combining the emerging technologies at this very discontinuing point in technology development. The partners bring world class technical expertise in the core areas that are crucial to the success of the project, specifically: embedded software systems, wireless and mobile technology, sensors, computer vision, software infrastructure/architecture, user interfaces and smart spaces. More information is available at the web sites: http://www.eecs.berkeley.edu/~eklund/projects/ITALH/ and http://www.summit06.dk/efter/worksessions/Morten_Kyng.pdf.

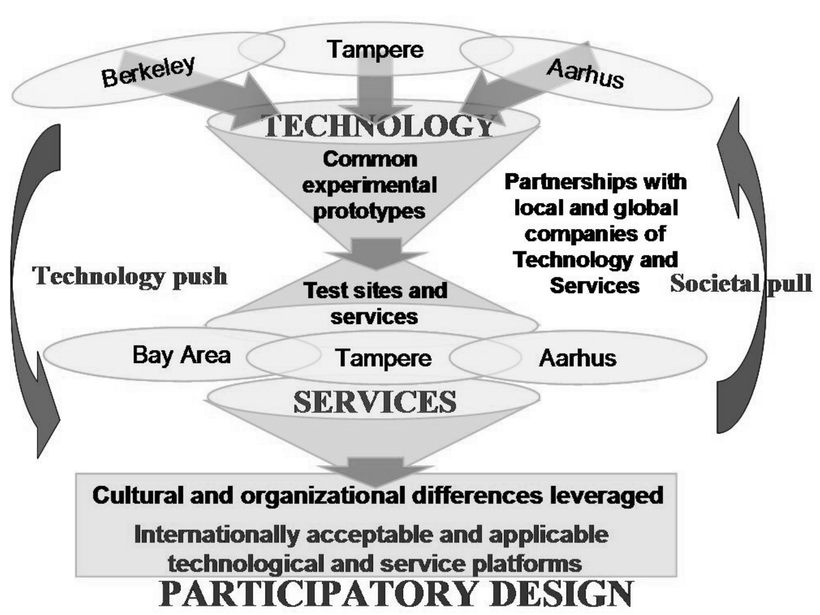


Fig. 3.1. Information Technology for Assisted Living at Home (ITALH) - technology transfer and collaboration.

In Finland two Tekes financed projects, UUTE (Smart Home in a Suitcase – Service Platform for Assisted Living and Safety; www.rgi.tut.fi/uute) and WISEPLA (Short-range wireless sensor platform for ambulatory and implantable applications; www.mit.tut.fi/wisepla), were created for the international ITALH project. The goal of the UUTE Tekes project within the ITALH is to study and develop technological and service platform that 1) support independent and safe living at home and especially patients recovery and rehabilitation at home and 2) supports the service providers and the personnel in their work towards heath and safety of the customer. Another WISEPLA project under ITALH focuses on development of wearable and implantable sensors for measuring mainly physiological parameters.

The research consortium has been active in participating European and other international collaboration projects. The consortium was a partner in two EU proposals filed in autumn 2004, but they failed to get trough. Furthermore, two more applications were filed in spring 2005 for 6th framework program. During the preparation of the project proposals the following partners were contacted and met during several meetings: Luleå University of Technology (Sweden), Tallinn University of Technology (Estonia), Fraunhofer IZM (Germany) and Polytechnic University of Catalonia (Spain). In Finland the cooperative partner was the University of Oulu.

The Wireless -project and the BIRCA-Biosensing Research Centre/Alliance were presented at the EU 6^{th} Framework Program Information Day on Ambient Assisted Living (AAL) in the Ageing Society on 30th of January 2006 by Jukka Vanhala. This resulted in a number of contacts and in two proposals for the call where the Wireless consortium was included.

The TULE project initiated international collaboration is expanding. Currently researcher MSc Mari Zakrzewski is at Berkeley. She will stay there until end of February 2007. Another researcher MSc Antti Vehkaoja will continue there from the beginning of January 2007. In addition, researchers MSc Sakari Junnila and MSc Harri Kailanto will visit Aarhus for three and one month, respectively.

4 Publications and Academic Degrees

Table 2. Publications and academic degrees produced in the project. Numbers of different types of publications are given along with the reference numbers. List of refereed journal articles are given in Section 6.1, refereed conference papers in Section 6.2, monographs in Section 6.3 and theses in Section 6.4.

Partner	Type of publication	2003	2004	2005	2006	**Total**	Publication numbers
TUT	Ref. journal art.	-	-	1	4	**5**	1-3, 4-5*
	Ref. conf. papers	-	3	6	7	**16**	6-18, 19*, $20\text{-}21^{+}$
	Monographs	-	-	-	-	**-**	
	Doctoral dissert.	-	-	-	1	**1**	30
	Licentiate degrees	-	-	-	-	**-**	
	Master degrees	-	3	1	4	**7**	22-29

* submitted, $^{+}$ accepted

5 Other Activities

Meetings

The Wireless Consortium has organized totally 13 consortium meetings during the project, so far. The kick-off meeting was held in August 14, 2003. A special research strategy meeting was organized in November 17, 2004 in the conference facilities of the Lapinniemi Spa.

Pasi Talonen and Tommi Majaus from Atrotech Ltd. (www.atrotech.com) visited the consortium meeting in January 13, 2004. Discussion was focused in the standardization and legal part of the design process of implantable devices and FDA Design Control Guidance.

Harri Heino from Bioretec Ltd. (www.bioretec.com) visited the consortium meeting in August 17, 2004. He presented the properties of sternum closure implants and introduced requirements for sensing the closing force and micro movements of sternum.

In addition to these two companies several other companies have been contacted and visited concerning wireless sensors during the planning of TEKES project applications in 2005.

August 2nd 2006 MIKA-project coordinator Mika Kamaja visited TUT/MIT to discuss about commercialization possibilities of the technology, especially the funding.

November 2003 meeting with Hermia business centre and a new start-up company Aniwell. Discussion about the technology to be developed and possibilities to apply in the business field of Aniwell.

Seminars and visits

Jukka Lekkala and Jukka Vanhala participated in the Session ”Innovation environments focusing on micro and nano technologies” of the Competitive City Regions – conference, Brussels, October 9-10, 2003.

Jukka Vanhala participated in the Elastomer Technology Seminar in November 7, 2003 and introduced our project. The seminar was organized by professor Kalle Hanhi from the Laboratory of Plastics and Elastomer Technology of TUT.

Minna Kellomäki and Jukka Lekkala gave comment statements in the TUTKAS (Tutkijoiden ja kansanedustajien seura) -seminar in the Finnish Parliament in November 12, 2003. TULE-programme and Wireless Consortium were shortly introduced.

Researchers of the project participated, "Wireless physiological sensors for ambulatory and implantable applications", Researcher seminar on Future Electronics Research Programme, TULE 2003-2006, Academy of Finland, Helsinki, Finland, 25.03.2004

All senior researchers of the Wireless Consortium participated and gave lectures in the Tampere Crossing Seminar in May 5, 2004.

Jari Hyttinen participated and gave a lecture in the HYVITE-seminar in May 27, 2004.

Juho Väisänen, Jarno Riistama, Jari Hyttinen and Jukka Lekkala participated in the 26th Annual International Conference of the IEEE EMBS in San Francisco, USA, 2004. The consortium presented 2 papers.

Part of the Wireless Consortium visited the Horse Center of Ypäjä in October 26, 2004. Seppo Hyyppä (vet.) made a stress test for a trotter using a treadmill. Muscle movements of the running horse was examined in order to find the optimal placement for a heart rate monitor implant. The horse ECG was recorded using both wired and wireless monitors.

Jari Hyttinen participated and gave a presentation: "Innovation alliance: Elder Tech for Home and Health." In the Danish Innovationsrådet åresmötet, Langelinie Pavillonen, Copenhagen (together with Morten Kyng, Aarhus University, Denmark and Mike Eklund University of California, Berkeley, USA)(http://innovationsraadet.dk/uplfiler/200410271018230.IA_TP_Oct_261004_Final.pdf?category_id=56), Copenhagen, Denmark, 26.10.2004

Jukka Lekkala participated and gave a lecture in the HYVITE-seminar in November 30, 2004.

Satu Arra participated and gave a lecture in the International Workshop on Wearable and Implantable Body Sensor Networks, 12-13.4.2005, Imperial College, London.

Jari Hyttinen gave a talk on TEKES organized USA Bay Area research opportunities workshop. Helsinki, Finland, 14.03.2005.

Researchers of the project participated, "Wireless physiological sensors for ambulatory and implantable applications", Mid-programme Researcher Seminar on Future Electronics Research Programme, TULE 2003-2006, Academy of Finland, Helsinki, Finland, 15.03.2005

The project group of RGI participated in the Second Tissue Engineering Symposium 12th April 2005, Tampere, Finland, and introduced the project the with poster presentation: Haltia, A.-M., Heinisuo, S., Kokko, K., Riistama, J. & Väisänen, J., "Wireless sensor technology for ambulatory and implantable human psychophysiological applications" II Tissue Engineering Symposium, Tampere, Finland, 12.4.2005.

Jukka Vanhala and Jukka Lekkala participated in the Smart Systems 2005, 4th International Conference of Smart Systems, 3-4.5.2005, Seinäjoki. The Wireless Consortium and the project were presented by a poster.

Jari Hyttinen and Juho Väisänen participated 5th International Conference on Bioelectromagnetism and 5th International Symposium on Non-invasive Functional Source Imaging within the Human Brain and Heart, Minneapolis, Minnesota, USA, 12.-15.05.2005. Juho Väisänen had as well a poster presentation in the conference.
Juho Väisänen participated and had a poster presentation in the Joint meeting of 5th

The consortium has participated in the TULE-program meeting for researchers in March 2004 as well as in TULE-half period seminar in March 2005. The consortium has presented posters of the project in both events.

Jari Hyttinen and Jukka Lekkala participated and gave lectures in the seminar Connections III Information and Communication Technologies for the Better Delivery of Health Care, University of California, Berkeley, CA, USA, 11.8.2005.

Juho Väisänen and Jari Hyttinen participated in the 13th Nordic Baltic Conference on Biomedical Engineering and Medical Physics, Umea, Sweden, 2005. Juho Väisänen presented a paper.

Minna Kellomäki and Jukka Lekkala participated and gave lectures in the Suomen Akatemian Tiedeaamiainen (Science Breakfast by Academy of Finland) – informative meeting for media, October 10th, 2005. Several interviews were made, and radio programs and news of the project released after the meeting.

Jari Hyttinen and Jukka Lekkala participated and organized a Special Session "Implantable Wireless Devices" in the 3rd European Medical & Biological Engineering Conference, Prague, Czech Republic, 2005.

Juho Väisänen and Jarno Riistama participated and gave lectures in the 3rd European Medical & Biological Engineering Conference, Prague, Czech Republic, 2005.

Jukka Lekkala participated and gave a lecture in the FinNano-Vision -seminar, TEKES, 13.2.2006.

Jari Hyttinen participated in the TEKES Finnwell program visit to MIT and Harvard University, Boston USA 7.2.-2.3.2006 and participated in the International Workshop on Wearable and Implantable Body Sensor Networks: April 3-5 at MIT Boston, USA.

Jukka Lekkala participated and gave a lecture in the Telemedicine and Telecare in Finland and Japan, JTTA seminar in Tokyo, May 12, 2006.

Jari Hyttinen and Juho Väisänen participated in the 33rd annual international conference of Computers in Cardiology, Valencia, Spain, 2006. Juho Väisänen also gave a lecture.

Jukka Lekkala participated and gave a lecture in the Biomedical Sensors - Foresight Workshop IV, 7 June 2006, Tampere, Finland.

Jari Hyttinen participated in the ICT for Bio-Medical Sciences conference, Brussels, 29th-30th June, 2006.

Satu Arra, Jukka Vanhala, Juho Väisänen, Jarno Riistama, Hanna Harjunpää and Jari Hyttinen participated in the 28th Annual International Conference of the IEEE Engineering in Medicine and Biology Society - EMBC, New York, USA, 30.8.-3.9.2006. Results of the project were presented in papers.

Jukka Lekkala participated and gave a lecture in the EuroBio 2006 Conference, Paris, France, 25 - 27 October, 2006.

Organization of seminars

Connection II Seminar, Forming new health & technology research partnerships, Tampere University of Technology, Tampere Finland. (http://websrv2.tekes.fi/opencms/OhjelmaPortaali/Kaynnissa/FinnWell/fi/Dokumenttiarkisto/Viestinta_ja_aktivointi/Seminaarit/Berkeley/Connections2_modeling_and_implant.pdf), Tampere, Finland, 03.01.2005

Institute of Biomaterials organized in cooperation with the Regea Institute of Regenerative Medicine of University of Tampere, Pirkanmaa University of Applied Sciences, and Tampere Graduate School in Biomedicine and Biotechnology three symposiums in tissue engineering in Tampere, Finland:

- The 1st International Tissue Engineering Symposium, 12 February, 2004,
- The 2nd International Tissue Engineering Symposium, 12 April, 2005, and
- The 3rd International Tissue Engineering Symposium, 4-5 May, 2006.

Survey

A questionnaire was submitted to altogether 154 doctors in Finland. The purpose was to be in contact with the users of the possible implantable devices and gain some knowledge about the needs there are in the field. The survey also served as an information channel towards the doctors about what the consortium is doing. The return percent was not astonishingly high, only 9.7 % which corresponds to 15 returned fill-in forms. What was however, delighting, was that all except one of the persons who returned the form, offered to cooperate with us.

6 Publications

6.1 Refereed Journal Articles

[1] J. Väisänen, J. Hyttinen, and J. Malmivuo, Focus of the Implantable Device's Measurement Sensitivity -Application of Half-Sensitivity Volume Concept, International Journal of Bioelectromagnetism, 1, vol. 7, pp. 240-242, 2005.

[2] Frisk, L., and Kokko, K., The effects of chip and substrate thickness on the reliability of ACA bonded flip chip joints, Soldering & Surface Mount Technology, vol. 19 (4), pp. 28-37, 2006.

[3] J. Väisänen, J. Hyttinen, J. Malmivuo, Finite Difference and Lead Field Methods in Designing of Implantable ECG Monitor, Med. Bio. Eng Comp, vol. 44 (10), pp. 857-864, 2006.

[4] J. Väisänen, J. Malmivuo, J.Hyttinen, Correlation between Signal-to-Noise Ratios and Region of Interest Sensitivity Ratios of Bipolar EEG Measurements, Med Bio. Eng Comp., submitted 10/2006.

[5] J. Väisänen, O. Väisänen, J. Malmivuo, J. Hyttinen, New Method for Analysing Sensitivity Distributions of Bioelectric Measurements, IEEE Trans. Bio. Med. Eng., submitted 12/2006.

6.2 Refereed Conference Papers

[6] J. Väisänen, J. Hyttinen, M. Puurtinen, P. Kauppinen and J. Malmivuo, Prediction of Implantable ECG Lead Systems by Using Thorax Models. Engineering in Medicine and Biology Society, Proceedings of the 26th Annual International Conference of the IEEE, San Francisco, CA, USA, Sep. 1-5, 2004, pp. 809-812.

[7] J. Riistama and J. Lekkala, Characteristic Properties of Implantable Ag/AgCl- and Pt-electrodes. Engineering in Medicine and Biology Society, Proceedings of the 26th Annual International Conference of the IEEE, San Francisco, CA, USA, Sep. 1-5, 2004, pp. 2360-2363.

[8] Hännikäinen, J., Järvinen, T., Vuorela, T., Vähäkuopus, K. & Vanhala, J., Conductive Fibres in Smart Clothing Applications, Proceedings of the 5th International Conference on Machine Automation, ICMA2004, Osaka University, Osaka, Japan, November 24-26, 2004, pp. 227-232.

[9] S. Arra, S. Heinisuo, and J. Vanhala, Acoustic Power Transmission into an Implantable Device, Proceedings of the 2nd International Workshop on Wearable and Implantable Body Sensor Networks, 12-13 April, 2005, Imperial College London, UK, 2005, 60-64.

[10] Kokko K., Haltia A-M., Harjunpää H. 2005. Elektroniikan pakkaaminen implantoitavissa laitteissa. Elektroniikan tuotanto- ja pakkaustekniikan konferenssi, Pori, Finland, 19-20 May 2005. pp. 92-96.

[11] J. Väisänen, J. Hyttinen, and J. Malmivuo, Development of Implantable Cardiac Measurement Device - Modeling Approach. 13th Nordic Baltic Conference on Biomedical Engineering and Medical Physics, Umeå, Sweden, June 13-17, 2005, pp. 99-100.

[12] Kokko K., Collander P. 2005 Historic and Future Trends in Miniaturisation of Electronics. The IMAPS Nordic Annual Conference, Tonsberg, Norway, 11-14 September 2005. pp.98-103.

[13] J. Väisänen, M. Ylinaatu, J. Hyttinen, and J. Malmivuo, Modelling Methods in the Implantable ECG Device Development, in proc. CD, 3rd European Medical and Biological Engineering and Computing Conference, 2005.

[14] Riistama, J., Lekkala, J., Väisänen, S., Heinisuo, J. and Hyttinen, J., Introducing a Wireless, Passive and Implantable Device to Measure ECG, IFMBE Proceedings. 3rd European Medical & Biological Engineering Conference IFMBE European Conference on Biomedical Engineering EMBEC´05. Vol., 11. Prague, Czech Republic. 20-25 November, 2005, pp. 1727-1983.

[15] J. Väisänen, O. Ryynänen, J. Hyttinen, J. Malmivuo, Analysing Specificity of Bipolar EEG Measurement, in proc. Engineering in Medicine and Biology Society, 2006. Proceedings of the 28th Annual International Conference of the IEEE, 2006, pp. 1102-1105.

[16] Heinisuo, S. & Vanhala, J., Wireless Platform for Multi-Channel Analog Measurements, Proceedings of the 28th Annual International Conference of the IEEE Engineering in Medicine and Biology Society - EMBC, New York, USA, 30.8.-3.9.2006, pp. 5908-5911.

[17] Riistama, J. and Lekkala, J., Electrode-electrolyte Interface Properties in Implantation Conditions, Proceedings of the 28th Annual International Conference of the IEEE Engineering in Medicine and Biology Society – EMBC. New York, USA, 30.8.-3.9.2006, pp. 6021-6024.

[18] J. Väisänen, J. Hyttinen, and J. Malmivuo, Analysing Specificity of a Bipolar ECG Implant to 12 Segments of the Left Ventricle, Computers in Cardiology 2006, Valencia, proceedings in press.

[19] Arra, S. & Leskinen, J. & Heikkilä, J. & Vanhala, J., Ultrasonic Power and Data Link for Wireless Implantable Applications. International Symposium on Wireless Pervasive Computing, 5.-7.2.2007, San Juan, Puerto Rico. Submitted 15.9.2006.

[20] Riistama, J. and Lekkala, J., Electrochemical noise properties of different electrode materials in different electrolytes, Body Sensor Networks Conference, Aachen, Germany, March 26-28, 2007, accepted.

[21] J. Väisänen, J. Hyttinen and J. Malmivuo, Optimizing Electrode Locations for Detecting Anterior Myocardial Infarction by Analysing Properties of the Sensitivity Distributions, Annual Conference of International Society for Computerized Electrocardiology,04/2007, accepted.

6.3 Monographs

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6.4 Doctoral, Licentiate, and Master Theses

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INTEGRATED POLYMER MICROSYSTEMS FOR FLUIDICS

Sami Franssila, TKK

Abstract

In this project novel polymeric microfluidic devices have been fabricated for analytical and health care applications. Different materials have been tested and integration of various fluidic functions on same microfluidic devices has been realized. These integrated microfluidic devices form the basis for miniaturized total analysis systems (μ-TAS). The project extends till 31.12.2007 and further improvements and applications are expected based on excellent results on the basic technologies investigated during the first two years.

From the studied materials epoxy polymer SU-8 was shown to be the best material for the integrated microfluidic devices. Structures can be fabricated with lithography and fluidic structures can be enclosed by patterned adhesive bonding. The phenomena of wafer-level bonding with SU-8 were investigated. Microchannel fabrication in SU-8 is excellent for cross-sectionally rectangular channels. Both depth and width of the channels can be varied from micrometers to millimeters on the same chip. High yield from the microchannel fabrication enables complex microfluidic networks or parallel fluidic systems. We have demonstrated three-layer SU-8 structures, but our adhesive bonding process using sacrificial substrate enables fabrication of even more complex multilayer fluidic systems.

The microchannel fabrication process is relatively easy and cheap. Therefore, SU-8 microchannels offers good platform for studying new types of microfluidic systems. Besides simple channels with wide range of geometries, SU-8 enabled us to integrate high aspect ratio pillars, electrodes and other additional functions to the microchips. Fluidic systems with various functions have been realized. In this project we have demonstrated the first electrophoretic separations using SU-8 microchips. SU-8 showed good material properties for electrophoretic separations. More detailed separation performance studies with SU-8 microchannels are currently on-going.

Electrospray ionization mass spectrometry (ESI-MS) from SU-8 microchips works well because of accuracy of ESI tip fabrication. Stability of the electrospray is good both with and without pressure assistance for driving the flow. Furthermore, SU-8 as a material is stable and compatible with most analytical solutions. Good results from the ESI-MS detection enabled us to further integrate separation systems with MS detection. Electrophoretic or chromatographic separations can be combined together with MS detection without major changes in the fabrication process. Integration of electrophoresis and ESI-MS detection has been demonstrated recently and further studies are underway.

1 Partners and Funding

1.1 Micro and Nanosciences Laboratory, Helsinki University of Technology

The research group consists of project leader docent Sami Franssila, graduate students Santeri Tuomikoski and Tero Ristolainen, and students Ville Jokinen and Eeva Läänilläinen.

1.3 Funding

Table 1. Funding of the project in 160 000 EUR in 2005-2007 (ca. 53 000 €/year). Internal funding consists of faculty salaries and operational expenditures provided by TKK. The funding provided by the Academy of Finland is shown in the table.

Partner	Funding Organization	2004	2005	2006	2007 (planned)	**Total**
TKK	Academy	0	53150	53710	53140	**160 000**
Total		**0**	**53150**	**53710**	**53140**	**160 000**

2 Research Work

2.1 Objectives and Work Plan

As stated in the work plan, "This research contributes to realization of novel integrated microfluidic devices, fabricated of new materials, and surface treated to provide performance advantage over existing devices."

2.2 Final Report: Common Themes and Collaboration

Various fabrication processes for making polymeric microfluidic chips have been studied. Lithographically definable epoxy polymer SU-8 was found to be exceptionally good structural material for microfluidic devices. Fully SU-8 microchannels were demonstrated in [1]. The goal of the paper was to find parameters for SU-8 bonding that are suitable for all possible structural dimensions of the microchannels. We found out that stresses caused by the microchannel-layer were the main reason for channel blocking noticed in earlier studies. Successful bonding for channel enclosure can be achieved by avoiding high stresses. This can be accomplished by selection of suitable bonding temperature slightly above SU-8 glass transition temperature and by controlled temperature ramp rates. However, besides the optimal process parameters the process requires also auxiliary structures designed next to the main channels. Microchannels up to 6 cm long with heights between 10 – 500 µm were fabricated successfully. The bonding method described in [1] is suitable for enclosing structures with various lateral dimensions on the same wafer with non-bonded area less than 5 % in wafer scale.

Furthermore, we invented a method how three-layer SU-8 chips can be removed from the substrates and those can be used as stand-alone microfluidic chips. The simplicity of fluidic inlet fabrication in fully SU-8 chips makes this fabrication scheme very attractive. By patterning the fluidic inlets to the first SU-8 layer and by releasing the structures from the substrate after bonding it is possible to fabricate fluidic inlets with lithographic accuracy. The fluidic inlet fabrication is problematic in most microfluidic device fabrication processes. The combination of low unintentional channel blocking and low non-bonded area enables fabrication of long microfluidic chips required in many microfluidic analysis applications. By application of auxiliary structures described in article [1], yield of 6 cm long microfluidic channels was 90 %; compared with 10 % yield without them, using identical bonding parameters. Initial fluidic experiments with capillary filling were made to test the usability of the channels. They showed promise of reproducible filling and reusability. Cross-section of 3-layer, fully SU-8 microchannel is shown in Figure 1 (a). Released fully SU-8 microfluidic channels are shown in Figure 1 (b)

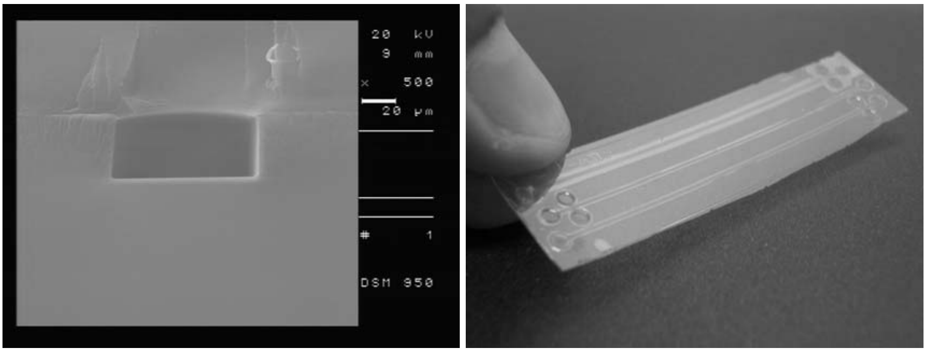

Figure 1 (a) Cross-section of microfluidic channel made fully of SU-8. (b) Released free-standing SU-8 microfluidic chip.

Fabricated microchannels were used for analytical separations by electrophoresis on microchip [2]. Since the first presentation of electrophoresis in a microchannel in 1992 the technique has become very popular separation method in the microchip world. Improved separation efficiency and reduced separation time in microscale have been driving the development of the technique. In article [2] fully SU-8 microchannels were used to determine the material suitability for electrophoresis. The paper was the very first measuring electroosmotic flow (EOF) in fully SU-8 microchannels. Measurements were compared with commercial glass microchips. SU-8 supports EOF mobility comparable to glass microchannels. This is very high value for polymeric microchannels and it promises fast separations in SU-8 microchannels. Clear pH dependence was noticed in SU-8 channels and furthermore the flow can be reversed in low pH values, which could enable new types of fluidic systems without need for additional coatings for the microchannels. The pH dependence of the EOF in SU-8 channel compared to commercial glass channel is shown in Figure 2.

Reproducible results from EOF measurements in SU-8 channels show that channel fabrication method developed in [1] is suitable for fluidic applications. The EOF values were double checked with zeta-potential measurements with SU-8 particles in buffer solution. The particles were fabricated on silicon wafer with sacrificial aluminum layer. Releasing of the particles was based on our earlier work on SU-8 microparticle fabrication.

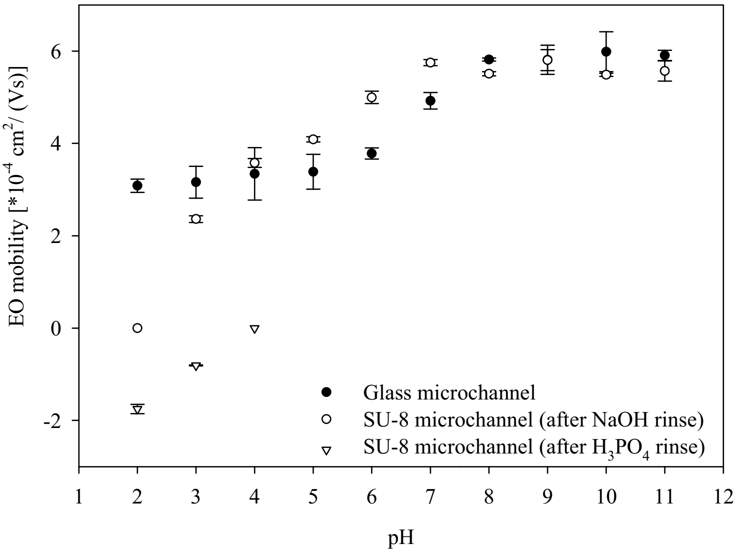

Figure 2 Results from EOF measurement in fully SU-8 microchannel at different pH

Electrophoretic separations of fluorescent markers [11] and real biomolecules like aminoacids and petides have been successfully demonstrated in our microfluidic channels [8]. Electrophoretic separation performance of our polymer microchips is comparable to commercial glass microchips. Separation of three different peptides is shown in Figure 3. We have also studied the chemical stability of SU-8 material in analytical applications. Our microchannels show very good chemical compatibility with the standard analytical chemicals. No absorption or deformations of microstructures were noticed in our microchannels due to chemicals.

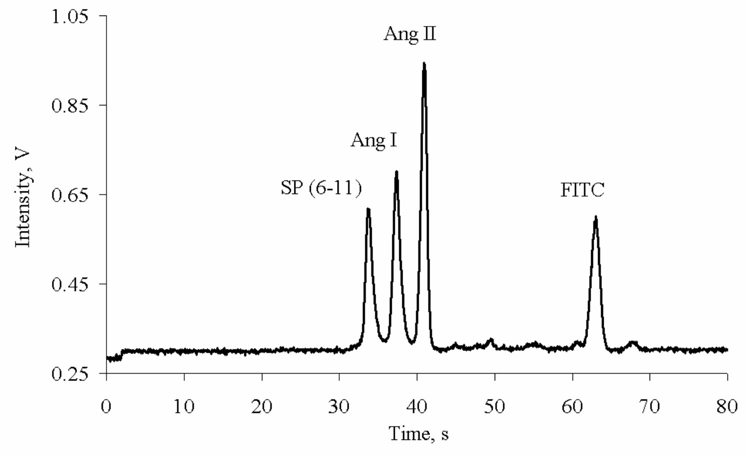

Figure 3. Separation channel made fully of SU-8, 20 µm *50 µm *85 mm, double-T injector. Separation of FITC-labelled Substance P (6-11), Angiotensin I and Angiotensin II 200 µM (each). 20 mM borate buffer (pH 10,0). 700 V/cm as separation voltage.

Electrospray ionization mass spectrometry (ESI-MS) is very sensitive detection method for microchip applications. Furthermore, detection can be done directly from real samples without labeling of the analytes. In fabrication of ESI emitter microchips for MS the biggest problem has been in patterning of nozzles accurately. Widely applied technique based on manual assembly of ESI capillaries is a laborious approach and the other used technique of spraying directly from blunt chip edge is not reproducible. In this paper we demonstrated the first enclosed SU-8 accurately defined ESI tips. Earlier versions have been open to air being prone to sample evaporation and poorly suitable for pressure driven flows. The process described in [1] was developed further to be able to pattern all three layers of SU-8. Masked exposure through the glass wafer and development via lanes enabled third layer patterning in a fast and simple process.

Tips with cross-sectional microchannel sizes between 10 μm *10 μm and 50 μm *200 μm were fabricated and tested successfully. MS tests were carried out with both pressure driven and electroosmotic flows, both showing stable performance. With electroosmotic sample transport stable spray is maintained in the timescale of tens of minutes, but with pressure driven flow stable functioning of the tip is extended to hours. Tips with microchannel cross-section of 50 μm * 80 μm and larger showed the most stable performance with RSD values repeatably less than 10 %. Due to accurately defined tip and hydrophobicity of the material Taylor cone and generated spray are well defined. SU-8 was shown to be a good material for analytical applications because no background was noticed from the material itself even at low m/z values. Fully released SU-8 microtips are shown in Figure 4.

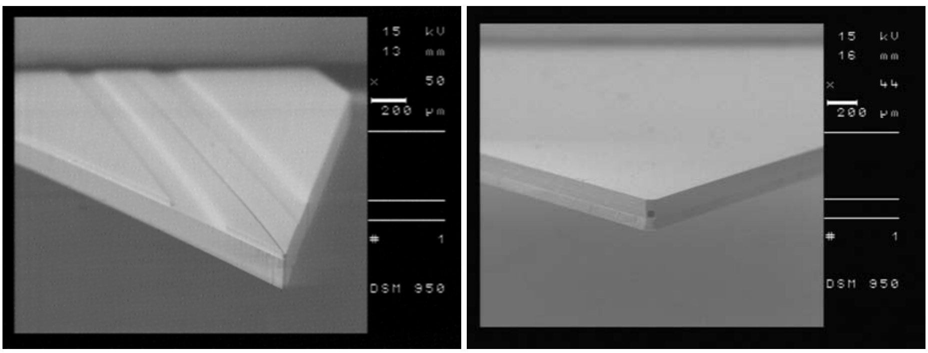

Figure 4 ESI tips made of SU-8; (a) Open channel before enclosure and (b) ready enclosed ESI tip.

We have integrated electrophoresis microchannel and electrospray ionization mass spectrometry on a same microchip [5]. The device is suitable for high sensitivity separation and detection of biomolecules. Earlier integration of separation channels with ESI-tips has been difficult to realize with fully microfabrication techniques. By using SU-8 the fabrication can be realized accurately and cost-effectively. Two examples of SU-8 electrophoresis – ESI-MS microchips are shown in Figure 5. In Figure 6 is shown the separation performance of the CE-ESI-MS microchips. The separation performance is very good compared to other microfabricated separation devices.

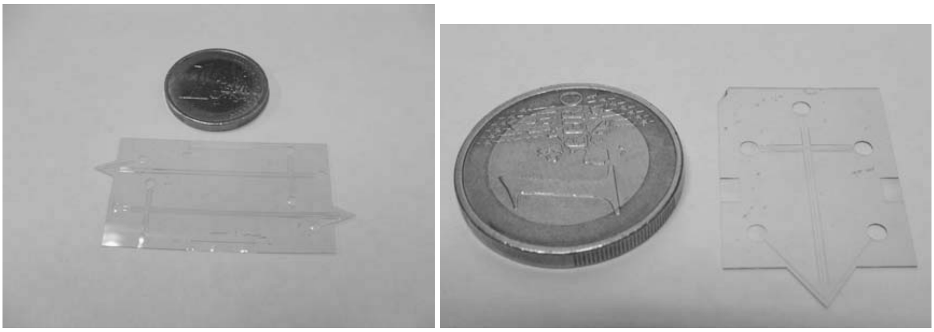

Figure 5. Examples of electrophoresis – ESI-MS microchips fabricated fully of SU-8.

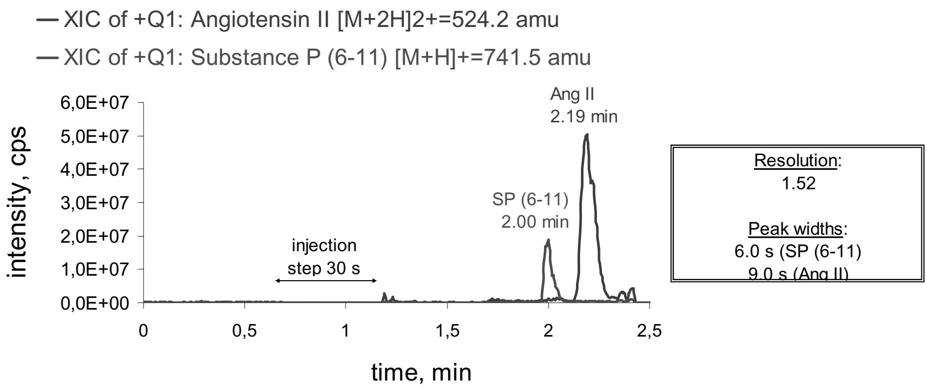

Figure 6. Separation of two peptides with online ESI-MS-detection in fully SU-8 microchips. CE-ESI-MS separation and detection of Angiotensin II and Substance P (6-11). Injected sample 112,5 fmol. Chip with auxiliary flow. Separation buffer 20 mM ammonium acetate + 40% methanol, auxiliary flow: methanol-water 80/20 + 1% acetic acid. Voltages: 5,5 kV Separation channel, 3,5 kV in auxiliary and 1 kV in MS

We have studied electrode integration to several polymeric microfluidic devices. Electrode integration to SU-8 microfluidic devices can be done more easily than with most other polymer microfabrication techniques. Because the microchips are fabricated fully lithographically electrode integration can be realized with basic microfabrication methods [10]. Platinum conductivity detection electrodes fabricated to SU-8 microchannels are shown in Figure 7.

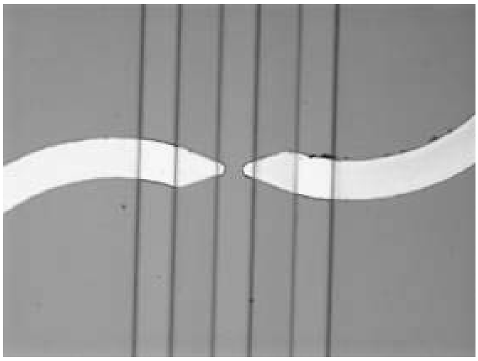

Figure 7. Platinum electrodes for conductivity detection in SU-8 microchannel

Metal patterning has also been studied with micro contact printing methods [14]. Micro and nanosized metal dots can be patterned on top of several substrates using microfabricated polymer master. The masters are fabricated of elastomeric polymer poly(dimethylsiloxane) PDMS. Binding of metals have been studied with and without binding chemicals. Self assembled monolayer (SAM) materials have been studied for linking the metals to the substrates.

Fabrication of microfluidic device for biomolecule separation is currently underway [15]. The device is based on capillary filling system and separation is based on surface interactions in patterned channels. The device is fabricated of SU-8 and different functionalities are made by various coatings technologies, including standard microfabrication methods and wet chemical treatments. Chemical binding of biomolecules to the SU-8 microchips has been studied also for other applications.

Mass spectrometry and capillary electrophoresis experiments have been carried out in active collaboration with the groups of profs. Risto Kostiainen and Tapio Kotiaho (University of Helsinki). This collaboration is continuing and several manuscripts have been submitted and are under preparation. Multidisciplinary approach to microanalytical devices has been found most fruitful, with publications in the leading journals in the field, like Lab Chip (impact factor 5.0), Sensors and Actuators B (if =2.6) and Electrophoresis (if = 3.7).

3 International Aspects

We have actively participated in the leading international conferences of the microfluidics field. International contacts have been made during these conferences. Santeri Tuomikoski has been in research collaboration with Louisiana State University, USA, working there twice during the project, studying polymer microfabrication techniques with embossing and imprinting methods. Visits have been made to: Massachusetts Institute of Technology MIT, USA; Tokyo University, Japan; Technical University of Denmark, Lund University, Technical University of Lausanne EPFL, University of Neuchatel and IBM Zürich.

4 Publications and Academic Degrees

Partner	Type of publication	2005	2006	2007	Total	Publication numbers
TKK	Ref. journal art.	3	1	4-5 ?		1-4
	Ref. conf. papers	5	3	3-4 ?		5-12
	Monographs	-	-			
	Doctoral dissert.	-	-	1		13
	Licentiate degrees	-	-			
	Master degrees	-	1	1		14-15

5 Other Activities

A popular science article “Mikrosuihkuja ja nanopisaroita” was published in magazine Prosessori (issue 11/2006). It has lead to an industrial contact and some preliminary experiments.

6 Publications

6.1 Refereed Journal Articles

1. Tuomikoski, S., Franssila, S., Free-standing SU-8 microfluidic chips by adhesive bonding and release etching, *Sens. Actuators A,* **120**, (2005), 2, 408-415

2. Sikanen, T., Tuomikoski, S., Ketola, R., Kostiainen, R., Franssila S., Kotiaho, T., Characterization of SU-8 for electrokinetic microfluidic applications, *Lab Chip,* **5**, (2005), 888-896.

3. Tuomikoski, S., Sikanen, T., Ketola, R., Kostiainen, R., Kotiaho, T., Franssila S., Fabrication of enclosed SU-8 tips for electrospray ionization mass spectrometry, *Electrophoresis*, **26**, (2005), 4691-4702

4. Saarela, V., Franssila, S., Tuomikoski, S., Marttila, S., Östman, P., Kotiaho, T., Kostiainen, R., Re-usable multi-inlet PDMS fluidic connector, *Sens. Actuators B*, **114**, (2006), 552-557

6.2 Refereed Conference Papers

5. [Tuomikoski, S., Sikanen, T., Ketola, R., Kostiainen, R., Franssila, S., Kotiaho, T., Integrated electrophoresis - electrospray ionization mass spectrometry microchip fabricated of SU-8, The 10th Annual European Conference On Micro & Nanoscale Technologies for the Biosciences, NanoTech 2006, November 2006, Montreux,

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9. Sikanen, T., Tuomikoski, S., Ketola, R., Kostiainen, R., Franssila, S., Kotiaho, T.,Optimization of analytical performance of microfabricated SU-8 emitters for electrospray ionization mass spectrometry, 17th International mass spectrometry conference, IMSC 2006, Prague

10. Tuomikoski, T., Ketola, R., Kostiainen, R., Kotiaho, T., Franssila, S., Fabrication and optimization of enclosed SU-8 tip structures electrospray ionization mass spectrometry, 9th international Conference on Miniaturized Chemical and Biochemical Analysis Systems, MICROTAS 2005, Boston, USA, 982-984

11. Sikanen, T., Korpisalo, I., Tuomikoski, S., Ketola, R., Kostiainen, R., Franssila, S., Kotiaho, T., Characterization of SU-8 microchannels for electrophoretic separations, 9th international Conference on Miniaturized Chemical and Biochemical Analysis Systems, MICROTAS 2005, Boston, USA, 1349-1351

12. Sikanen, T., Korpisalo, I., Tuomikoski, S., Ketola, R.A., Kostiainen, R.,Franssila, S., Kotiaho, T., Electrophoretic separations of pharmaceutical compounds in microchannels composed of SU-8 polymer. PharmaSciFair, Pharmaceutical Sciences Fair & Exhibition 12.-17.6.05 Nice, France.

6.3 Monographs

6.4 Doctoral thesis

13 S. Tuomikoski, Fabrication of SU-8 microstructures for analytical microfluidic applications. Doctor of Science in Technology dissertation, Department of Electrical and Communications Engineering, Helsinki University of Technology, 2007.

6.5 Masters thesis

14. E. Läänilläinen: Soft lithography for surface micropatterning, 2006

15. V. Jokinen: Capillary filling of complex microchannels (expected date: February 2007)

7 Other References

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17. Journal manuscripts in preparation:

- Sikanen, T., Zwinger, T., Tuomikoski, S., Franssila, S., Lehtiniemi, R., Fager, C.-M., Kotiaho, T. Pursula, A, Temperature modeling and measurement of an electrokinetic separation chip
- Sikanen, T., Tuomikoski, S., Ketola, R., Kostiainen, R., Franssila, S., Kotiaho, T. Analytical performance of microfabricated SU-8 emitters in electrospray ionization mass-spectrometry
- Sikanen, T., Heikkilä, L., Tuomikoski, S., Ketola, R., Kostiainen, R., Franssila, S., Kotiaho, T. Biomolecule electrophoretic separations in fully SU-8 microchannels

New materials and structures for semiconductor gas sensors (NEWGAS)

Pekka Kuivalainen[1] and Vilho Lantto[2].

Abstract

The aim of the present research project was to develop new advanced gas sensors with enhanced performance based on new materials such as epitaxial tin dioxide, porous silicon and tungsten trioxide nanoparticles together with new micromechanical air bridge structures. The research work utilized the state of the art measurement systems for gas sensor materials based, e.g., on the Kelvin probe techniques, which allow in situ studies of the gas reactions at the sensor surfaces. The new epitaxial and layered semiconductor materials have been chosen to maximize the sensitivity and the long-term stability. On the other hand, the new micromechanical air bridge structures and, similarly, the possibility for sensing without heating with WO_3 nanoparticles allow a significant reduction in power consumption, which is vitally important in portable applications. Both the growth of the new materials and the demanding characterization techniques were based on the previous experience of the present research consortium on the epitaxy of semiconductor thin films and the extensive studies of the polycrystalline tin dioxide as a gas sensor material.

1 Partners and Funding

1.1 Electron Physics Laboratory, Helsinki University of Technology

The research group consisted of the subproject leader professor Pekka Kuivalainen, senior researcher Dr. Sergey Novikov, and a postgraduate student Mikael Kroneld.

1.2 Microelectronics and Materials Physics Laboratories, University of Oulu

The research group consisted of subproject leader professor Vilho Lantto and postgraduate students Sami Saukko and Luis Reyes. The research has been done also in a close co-operation with the research group of Professor C.G. Granqvist at the Uppsala University (postgraduate student Peter Heszler and Dr. Anders Hoel), and with Professor Janos Mizsei from the Budapest University of Techology and Economics. Dr. Johannes Frantti from the Tokyo Institute of Technology has also participated in the research.

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[2] Microelectronics and Materials Laboratory, University of Oulu, FIN-90014, Oulu Finland, P.O.Box 4500, FIN-90014, Universtity of Oulu, Finland

1.3 Funding

Table 1. Funding of the project in 1000 EUR in 2003-2006

Partner	Funding Organisation	2003	2004	2005	2006	**Total**
HUT	Academy	14.860	29.720	28.840	16.580	**90**
OU	Academy	22.238	31.870	21.000	14.892	**90**

2 Research Work

2.1 Objectives and Work Plan

The aim of the present research consortium was to develop and utilize new materials and structures in the fabrication of semiconductor gas sensors showing enhanced stability and reduced power consumption. They could be realized by using an epitaxial growth of semiconductor thin films and nanocrystalline layered WO_3 films and by a proper choice of doping and catalyst additives, and by reducing the size and layout of a heating element with micromechanical bridge structures allowing a decrease in power consumption. Also the gas sensor characterization techniques based on the Kelvin probe method was developed and utilized in *in situ* measurements of the gas reactions at the semiconductor surfaces.

In the first phase of the project the fabrication techniques for the novel gas sensing materials such as monocrystalline SnO_2 and nanoparticle WO_3 were developed. Also the Kelvin probe technique was developed in the new scanning equipment, in which a complicated gas system was connected. After an extensive characterization of the grown materials including tens of samples the main task was the study the responses of the fabricated gas sensors to about ten different gases including CO, Ethanol, NO_2, H_2S and CHOH (formaldehyde).

2.2 Final Report: Common Themes and Collaboration

The present research project started in the beginning of July 2003. The main goal, which was to grow high quality gas sensing materials, has been achieved in the case of tin dioxide. By adjusting the growth parameters we are able to grow either polycrystalline nanoparticle thin films or monocrystalline thin films. Extensive characterization of the grown thin films has been carried out including, e.g., reflection high energy electron diffraction (RHEED), X-ray diffraction (XRD), atomic force microscope (AFM), Hall-effect, and conductance measurements in close collaboration between the consortium partners, which has produced two joint publications [2 and 3]. Oxygen adsorption-desorption kinetics at the tin oxide surface has been studied experimentally using

temperature-programmed desorption method together with the conductance measurements. Also simultaneous Kelvin probe and conductance measurements during heating and cooling in different ambient atmospheres were used to characterize the monocrystalline $SnO_2(101)$ surface after various surface treatments.
Due to a cut in the planned budget the fabrication of the heated substrates with microbridge structures was transferred to an industrial project. These structures are now available in Micronova.

2.3 Final Report: Electron Physics Laboratory, HUT

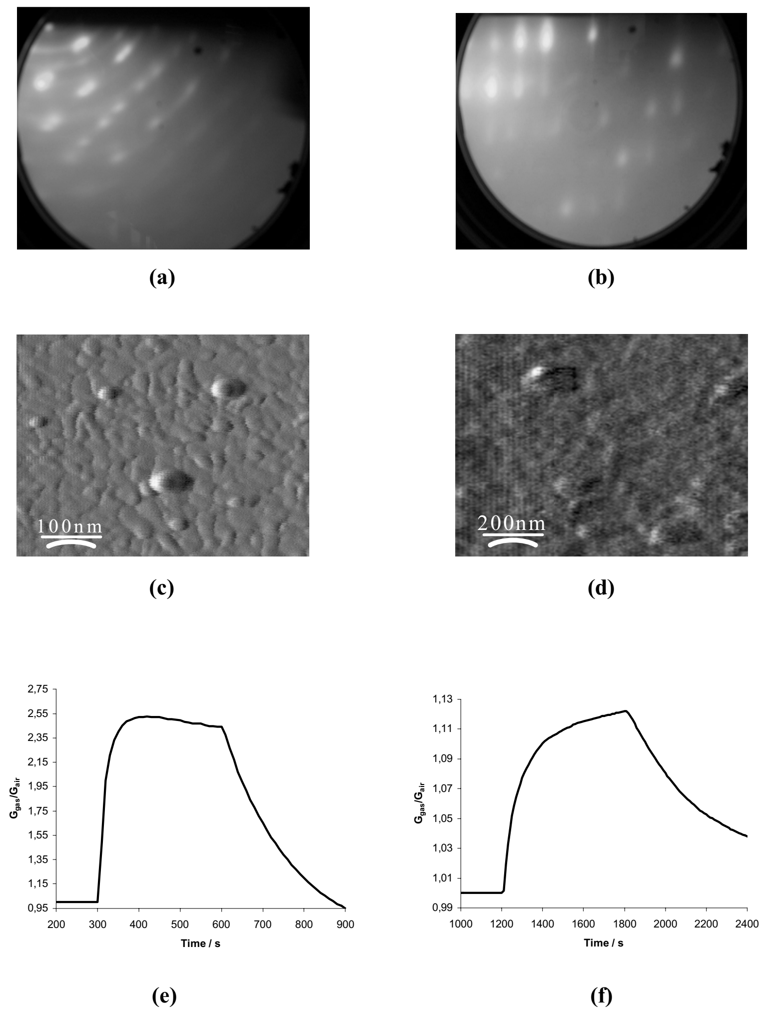


Fig. 1. A comparison between two samples grown at different temperatures; a) RHEED image of a clearly polycrystalline sample, b) RHEED image of a monocrystalline sample, c) and d) AFM images of the corresponding samples, e) and f) conductivity responses towards an exposure of 1000 ppm hydrogen at 400 °C.

Our research results on mono- and nanocrystalline SnO_2 thin films are very promising. X-ray diffraction results confirmed that all the thin films grown are highly oriented along the surface as only one peak in addition to the substrate could be seen in the scan. A comparison between samples of different crystalline quality is shown in Fig. 1.
Three-dimensional diffraction spots and rings on the RHEED image obtained from sample in Fig. 1. a) indicate a rough surface and a polycrystalline nature of the film. Sample grown at higher temperature (Fig. 1. b)) gives an image with elongated spots, which indicates that the electron beam hits a monocrystalline region. The AFM inspection confirms that the crystalline quality in the case of higher growth temperature is clearly better, see Fig. 1 c) and Fig. 1 d).
As is evident from Fig. 1. e) and Fig. 1. f), the film of better crystalline quality shows lower response towards the test gas, which may be expected, due to the reduced number of grain boundaries. The rise time for the film of smaller grains is shorter, but the decrease in the response during the gas exposure is evident in the case of smaller grains. Results allow and encourage us to further optimize the growth parameters and thus the structural characteristics of the sensing films.
The SnO_2 thin films were typically grown on an *r-cut* sapphire substrate, with very encouraging results. However, to further optimise the growth, we also fabricated monocrystalline SnO_2 on sapphire substrates with a particular off-cut from the *r*-plane, which provided us even better film qualities due to the optimisation of three-dimensional growth.

So, we have succeeded in the growth of the single crystal tin dioxide thin films on sapphire substrates, which was one of the main goals in the project plan. The samples have been grown by using molecular beam epitaxy, MBE. For comparison also polycrystalline tin dioxide thin films have been grown. Altogether the number of succesful sample growth runs was over 20. Some of these samples are listed in Table 1 below. At Oulu University we have carried out gas response measurements for hydrogen, sulphur hydrogen and carbon monoxide. In Otaniemi we have measured also responses, e.g., to ethanol. Based on the results of these measurements we can state that the resistivity of the samples reacts strongly to the gas exposure. The measured sensitivity is higher in polycrystalline samples, but the stability seems to be better in single crystal thin films. Recently we have fabricated sensor material including catalyst materials such as Pt. The monocrystalline material differs from the nanocrystalline material in many respects: Not only the AFM and XRD analysis but also the charge carrier mobility is an order of magnitude higher in the monocrystalline case (see the **bold** numbers in Table 1). This is a good indication of the higher crystal quality, since the mobility is a very sensitive parameter to the crystal defects.

Table 1. Nano- and monocrystalline SnO_2 samples grown by using MBE.

Sample	Growth temperature ^{0}C	Target	Thickness /nm	Mobility/ cm^2/Vs	Carrier concentration/ cm^3	Conductivity/S/cm
1	550	SnO_2	100	1.0	$7*10^{17}$	0.12
2	420	Sn	100	7.6	$3*10^{17}$	0.33
3	460	Sn	100	2.6	$5*10^{16}$	0.021
4	550	SnO_2	100	NA	NA	NA
5	420	Sn	100	3.9	$7*10^{17}$	0.44
6	520	SnO_2	100	NA	NA	NA
7	390	Sn	100	11.7	$2*10^{18}$	4.1
8	420	SnO_2	100	3.4	$4*10^{18}$	2.4
9	420	SnO_2	30	2.9	$7*10^{17}$	0.34
10	**420**	**SnO_2**	**30**	**30**	**$3*10^{16}$**	**0.15**
11	420	SnO_2	30	4.1	$7*10^{18}$	4.4
12	420	SnO_2	30	2.2	$2*10^{18}$	0.63
13	570	SnO_2	30	NA	NA	NA
14	570	SnO_2	30	3.6	$5*10^{17}$	0.27
15	520	SnO_2	30	NA	NA	NA

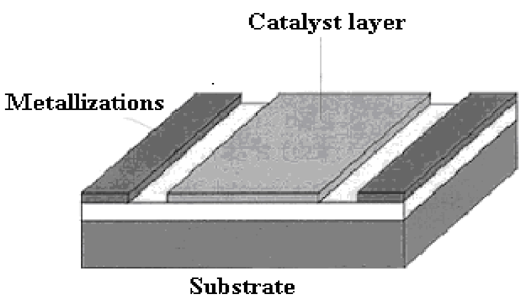


Fig.2. Gas sensor structure for MBE grown SnO_2 .

Fig. 2 shows the simple device structure used in the gas sensing testing.

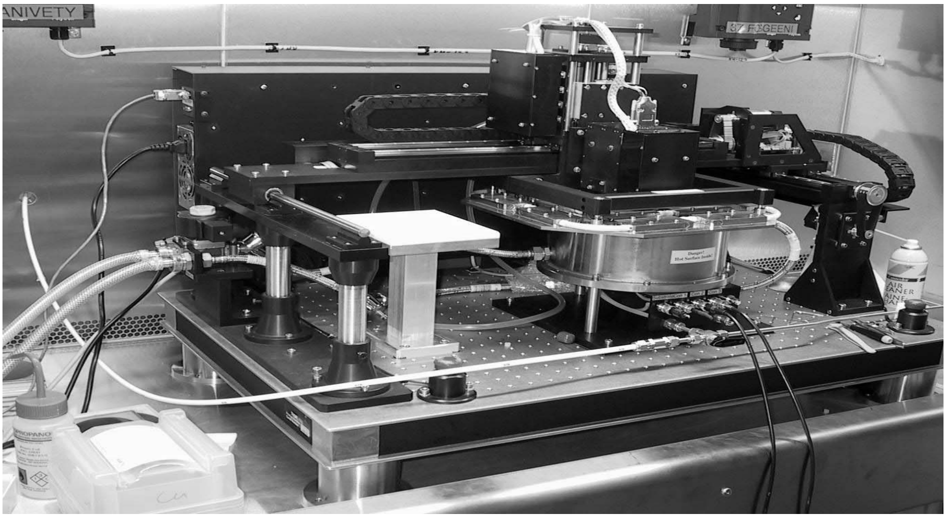


Fig.3. Scanning Kelvin probe for surface potential measurements.

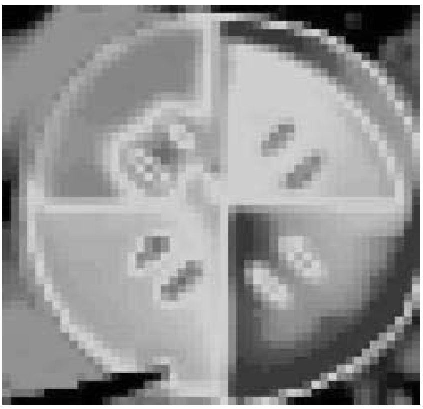
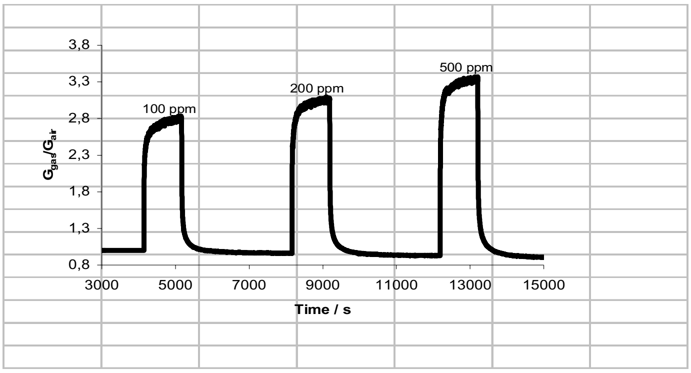


Fig.4. Measured surface potentials for 4 different samples: Bare tindioxide (the upper left corner), with a Pt catalyst layer (the upper right corner), with a Pd catalyst layer (the lower left corner), and with a Ni catalyst layer.

A new gas measurement system was built at HUT, which includes gas sources for over ten different gases and a new scanning Kelvin probe to measure the gas responses of the sensor materials (Fig.3). The gas responses for different gas sensing materials can now be measured simultaneously, as shown in Fig.4.



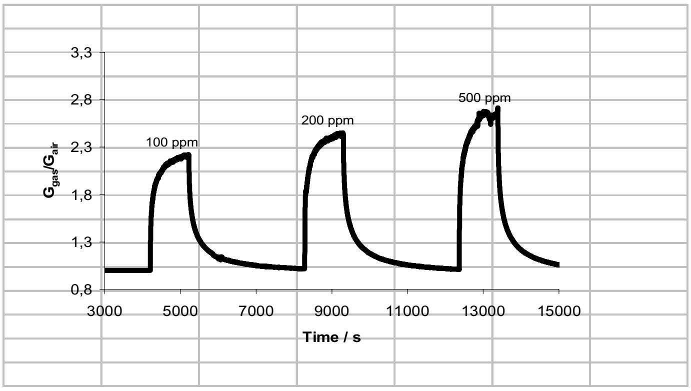


Fig.5. Gas responses (changes in relative conductance) for ethanol in the cases of moncrystalline (upper figure) and nanocrystalline SnO_2 .

Typically the sensitivity of the monocrystalline SnO_2 was smaller than in nanocrystalline case (see Figs.1 (e) and (f)) due to the smaller effective surface area. However, in some cases the monocrystalline layer was more sensitive as shown in Fig.5 for ethanol.
Although we did not carry out systematic long term stability tests, we obtained a good indication of a better stability in our monocrystalline samples as compared to the commercial devices, since in our samples there was no drift in the gas response during the long exposure time.

2.4 Final Report: Microelectronics Laboratory, OU

Traditionally, semiconductor gas sensors, and in particular gas sensors using SnO_2 as a sensing material, are based on polycrystalline thin or thick films. Sensing mechanisms of these types of sensors have been widely studied and are quite well understood. The novel approach is to use monocrystalline SnO_2 thin film as the sensing layer. The intergrain potential barriers that are mostly responsible for the sensing mechanism in polycrystalline films are missing in monocrystalline films. With monocrystalline structure, however, it may be possible to overcome some of the problems that are typical for polycrystalline sensors such as long term stability, response and recovery times and variation in electrical properties from sensor to sensor, especially in the case of thick film sensors.

We have studied different surface phenomena on SnO_2 surfaces using both monocrystalline and polycrystalline samples with various experimental characterization techniques, such as TPD, surface potential (Kelvin probe) and conductance measurements in different ambient conditions in order to understand better the sensing mechanism in monocrystalline films (Publication No. 3). So far, the results show that the monocrystalline film behaves very differently compared to the polycrystalline samples. Stability with both time and temperature is better and overall characteristics of the different sensors are more alike. Even though the premilinary testing shows that the sensitivity is lower, as expected, in the case of monocrystalline films as compared to the polycrystalline films, the increased overall stability of the new structure makes it, as a whole, a promising structure for gas sensors. Monocrystalline film makes it also easier to study the possible influence of electrodes on the sensitivity and selectivity (Publication No. 9).

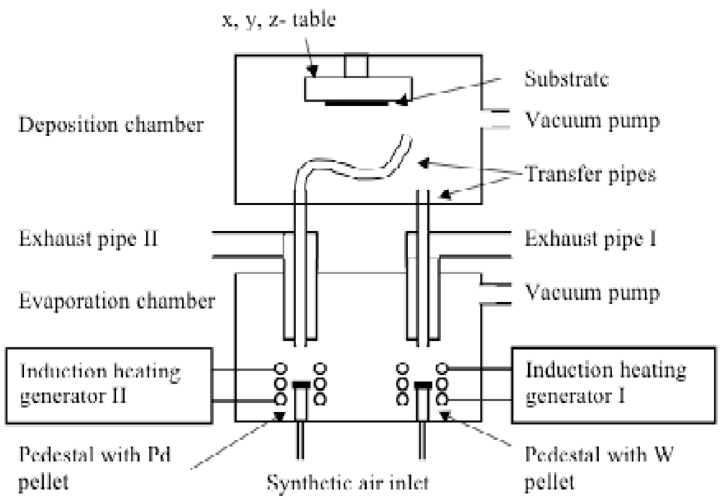


Fig. 6. Schematic diagram of the ARGD unit with two separate induction heaters.

The project made it also possible to continue in OU the preliminary research on the possibility to use nanostructured tungsten trioxide, WO_3, films for gas sensing applications in co-operation with research groups in the Uppsala University (UU) and in the Technical University of Lima, and also with researchers in Hungary. Advanced Reactive Gas Deposition (ARGD) unit in UU was used to fabricate nanostructured WO_3 powder and films with a crystal structure different from the bulk crystal structure at temperatures between room temperature and about 600 K. The ARGD unit was developed further to deposit also catalytic additives like Au and Pd nanoparticles simultaneously with the deposition of nanostructured WO_3 films by using two separate induction heaters in the system (Fig. 6, Publications No. 1, 5 and 8). Figure 7 shows a transmission electron micrograph (TEM) depicting a cross-section of an as-deposited WO_3 sample.

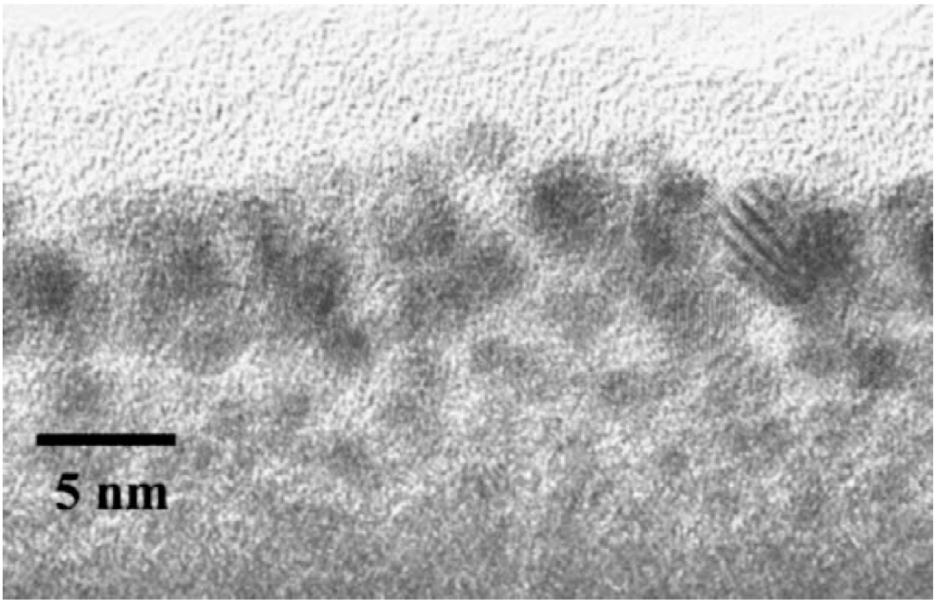


Fig. 7. Transmission electron micrograph depicting a cross-section of an as-deposited WO_3 sample.

The symmetry of WO_3 is lowered from that of the cubic ReO_3 structure by two distortions: tilting of WO_6 octahedra and displacement of tungsten from the center of its octahedron, as is shown in Fig. 8 where the crystal structure of the low-temperature monoclinic ε-WO_3 phase (from 0 up to 230 K in bulk WO_3) is shown in the direction of view [100].

Direction of view [100]

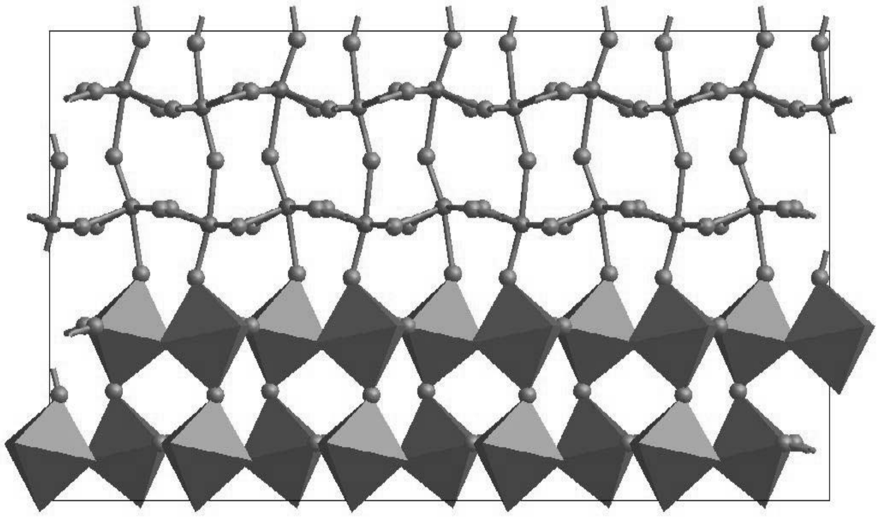


Fig. 8. Crystal structure of the low-temperature monoclinic phase of WO_3 (ε-WO_3).

The structure is ferroelectric, whereas the highest symmetry tetragonal α-WO_3 above about 1010 K in the bulk WO_3 is antiferroelectric. Physical properties of the different crystal structures of WO_3 depend crucially on the details of the distortions and tilting of oxygen octahedra in the structure. It was found that the crystal structure of WO_3 nanoparticles depends on the size of particles and is different from the room-temperature monoclinic structure of the bulk WO_3 at temperatures from room temperature up to about 600 K, as is shown from the x-ray and Raman results in Fig. 9. Many results of different characterization methods like x-ray and neutron diffraction, Raman scattering, TEM, SEM, AFM, XPS and Kelvin method together with different electrical and optical studies made it possible to understand both the crystal structure and band structure, and also the electrical conduction mechanism of the WO_3 nanoparticles.

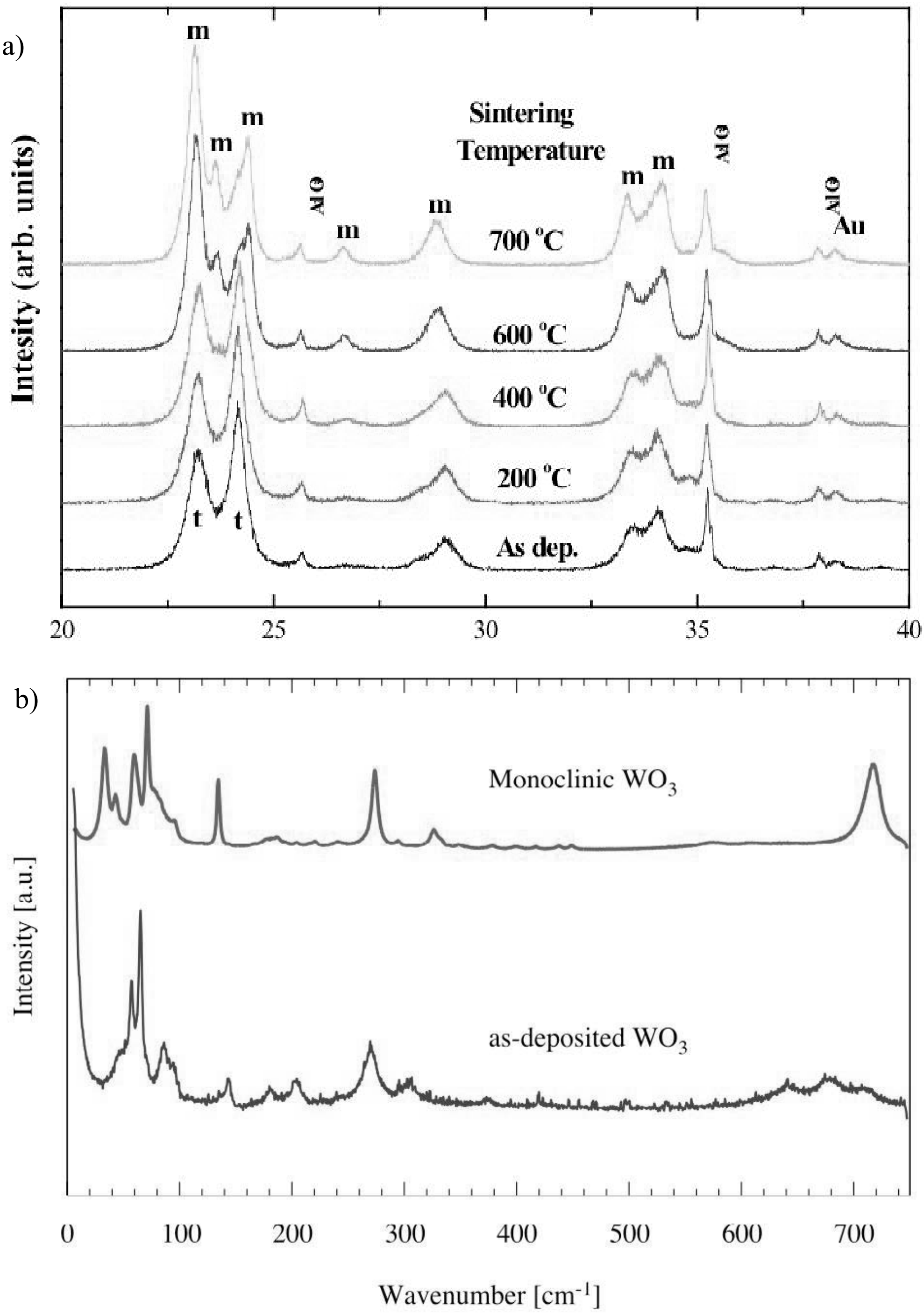


Fig. 9. a) XRD from Au-activated WO_3 nanoparticle film both as-deposited and sintered in the range of 200 °C to 700 °C. b) Raman spectra of commercial WO_3 powder (monoclinic) and as-deposited WO_3 nanoparticle film measured at room temperature.

Gas response properties of nanostructured WO_3 films as pure and modified with different additives were studied at exposures to various gases at different concentrations in air at room-temperature operation and also as a function of temperature (Fig. 10, Publications No. 1, 4, 5, 8). The interfering effects of humidity where also studied. It was possible to improve the excellent sensitivity of WO_3-based samples towards H_2S at room-temperature operation by modifying the microstructure of the sensing layer using different growth parameters. Further, by adding small amounts of noble metal nanocatalysts into the sensing layer it was possible to improve the sensitivity down to the sub ppm level at H_2S exposure. Research with porous silicon has also continued in the Microelectronics Laboratory at OU and some test measurements on the gas response of these samples have been also done by professor Mizsei using both the Kelvin probe and photovoltage measurements.

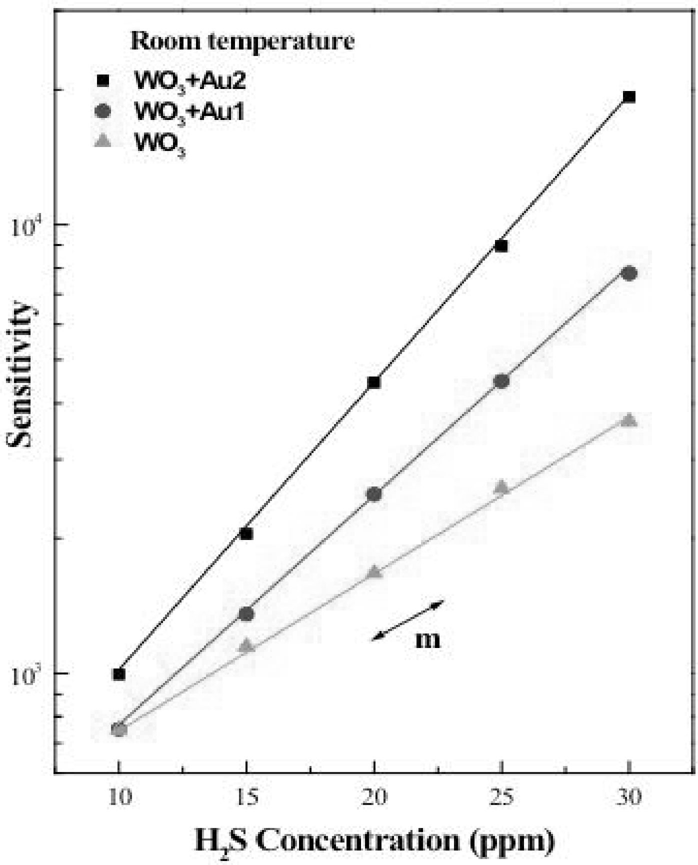


Fig. 10. Sensitivity as a function of H_2S concentration at room temperature for pure and Au-activated WO_3 films sintered at 300 °C

3 International Aspects

The new scanning Kelvin probe applicable in a gas atmosphere was planned together with a Hungarian group headed by Dr. Tibor Pavelka at Semilab Ltd. During the project Professor Janos Mizsei from the Budapest University of Technology and Economics has visited both the Microelectronics Laboratory at OU and the Electron Physics Laboratory at HUT. As a result a joint publication has been written ([3]; see the list below). There has been also a close research co-operation in the research with layered nanocrystalline WO_3 samples between researchers in the Microelectronics Laboratory at OU and in the Ångström Laboratory at the Uppsala University (research group of Professor Granqvist). Luis Reyes from the Technical University of Lima, Peru has been working as a postgraduate student in OU (supervisor Prof. Lantto) and in UU (supervisor Prof. Granqvist). Dr. Johannes Frantti from the Tokyo Institute of Technology has participated also in the experimental characterization of the structure of the WO_3 sensing films using Raman spectroscopy.

4 Publications and Academic Degrees

Table 2. Publications and academic degrees produced in the project.

Partner	Type of publication	2003	2004	2005	2006	**Total**	Publication numbers
HUT	Ref. journal art.	-	-	1	1	**2**	2, 3 (joint publications with OU)
	Ref. conf. papers	-	-				
	Monographs	-	-	-		**-**	-
	Doctoral dissert.	-	-	-		**-**	-
	Licentiate degrees	-	-	1		**1**	12
	Master degrees	-	-	-			-
OU	Ref. journal art.	1	4	2		**8**	1,2,3,4,5,6,7,8,9
	Ref. conf. papers	1	-	-		**1**	10
	Monographs	-	-	-			-
	Doctoral dissert.	-	1	-		**1**	13
	Licentiate degrees	-	-	-			-
	Master degrees	-	-	-	1	**1**	11

5 Other Activities

The results of the project have been presented to Dr. Mikko Utriainen at Environics Ltd. in several meetings. Two new industrial gas sensor projects were started recently in Micronova. In these projects the results of the present academic project can be utilized.

6 Publications

6.1 Refereed Journal Articles

[1] L.F.Reyes, A.Hoel, S.Saukko, P.Heszler, V.Lantto, and C.G.Granqvist, Gas sensor response of pure and activated WO3 nanoparticle films made by advanced reactive gas deposition., *Sensors and Actuators* B: Chemical, **117** (1):128-134, 2006.

[2] M.Kroneld, S.Novikov, S.Saukko, P.Kuivalainen, P.Kostamo, and V.Lantto, Gas sensing properties of SnO_2 thin films grown by MBE, *Sensors and Actuators*, **B118**: 110-114, 2006.

[3] S. Saukko, U. Lassi, V. Lantto, M. Kroneld, S. Novikov, P. Kuivalainen, T.T. Rantala, and J. Mizsei, Experimental studies of O_2-SnO_2 surface interaction using powder, thick films and monocrystalline thin films, *Thin Solid Films*, **490**: 48-53, 2005.

[4] L.F. Reyes, S. Saukko, A. Hoel, V. Lantto, and C.G. Granqvist. Structure engineering of WO3 nanoparticles for porous film applications by advanced reactive gas deposition. *Journal of European Ceramic Society*, **24**, Issue 6:1415–1419, 2004.

[5] A. Hoel, L. F. Reyes, S. Saukko, P. Heszler, V. Lantto, and C. G. Granqvist. Gas sensing with films of nanocrystalline WO3 and Pd made by advanced reactive gas deposition. *Sensors and Actuators B: Chemical*, **105**(2):283–289, 2005.

[6] V. Lantto, S. Saukko, N.N. Toan, L.F. Reyes, and C.G. Granqvist. Gas sensing with perovskitelike oxides having ABO3 and BO3 structures. *Journal of Electroceramics*, **13**:721–726, 2004.

[7] A. Hoel, L. F. Reyes, P. Heszler, V. Lantto, and C. G. Granqvist. Nanomaterials for environmental applications: novel WO3-based gas sensors made by advanced gas deposition. *Current Applied Physics*, **4**(5):547–553, 2004.

[8] L.F. Reyes, S. Saukko, A. Hoel, V. Lantto, and C.G. Granqvist. Improved gas response at room temperature of activated nanocrystalline WO3 films. *Physica Scripta*, **T114**:240–243, 2004.

[9] S. Saukko and V. Lantto, Influence of electrode material on properties of SnO_2-based gas sensor, Thin Solid Films, 436:137-140, 2003

6.2 Refereed Conference Papers

[10] L.F. Reyes, S. Saukko, A. Hoel, V. Lantto and C.G. Granqvist, H_2S sensing with nano-structured WO_3 films in different oxygen atmospheres, Proc. (CD-ROM) 17th European Conference on Solid-State Transducers (Eurosensors XVII), Sept. 21-24, 2003, Guimaraes, Portugal, pp 859-860.

6.3 Monographs

6.4 Doctoral, Licentiate, and Master Theses

[11] L.F. Reyes, Sensores de gas basados en nanoparticulas de WO_3 sensibles a H_2S a temperatura ambiente (Gas sensors based on WO_3 nanoparticles sensible to H_2S at room temperature), Universidad Nacional de Ingenieria, Lima, Peru, 2006 (Master Thesis)

[12] M.Kroneld, Gas sensing properties of mono- and polycrystalline tin dioxide thin films grown by MBE, HUT 2005, 90 pages. (Licentiate thesis)

[13] A. Hoel, Electrical Properties of Nanocrystalline WO_3 for Gas Sensing Applications, Acta Universitatis Upsaliensis. *Comprehensive Summaries of Uppsala Dissertations from the Faculty of Science and Technology* 948. Uppsala (2004) 86 pp. (Doctoral thesis)

7 Other Outputs

- An invited lecture with the title "On some structural effects of transition metal oxides with relevance to gas sensing: WO_3 as an example oxide" was given by V. Lantto 12.2.2004 in the Yamazoe Laboratory at the Kyushu University, Fukuoka, Japan.
- An oral lecture with the title "Gas sensing with nanocrystalline tetragonal WO_3 films" was given by V. Lantto in the 9th International Conference on Electroceramics & their Applications, 31.5.-3.6.2004, Cherbourg, France.
- An invited plenary lecture with the title "Some structural and electronic aspects on gas sensing with transition metal oxides" was given by V. Lantto in the Opening Session of the Semiconductor Gas Sensors (SGS´2004) Seminar, 19.-22.9.2004, Ustron, Poland.

NOVEL ELECTROACOUSTIC SOLUTIONS FOR MICROMECHANICAL RADIOS (MIRA)

Antti V. Räisänen[1], Timo Veijola[2], Ilkka Tittonen[3], Matti Kaivola[4], Heikki Seppä[5]

Abstract

The MIRA project aimed at developing a novel, highly integrated radio transceiver with the help of MEMS technology. With MEMS (micro-electro-mechanical systems) technology, mechanical signal processing can be integrated on the same chip with CMOS electronics. For radio systems this is desirable since many components of common radio architectures can benefit from the properties of MEMS, such as small size and low loss. Such components include switches, filters, mixers, local oscillators, phase shifters and variable capacitors. On the other hand, MEMS can enable totally new radio architectures with novel components, such as extremely long delays in a small volume, and where several functions are performed in a single component, such as filtering and mixing.

During the MIRA project, several components have been modelled, designed, fabricated and characterized in close collaboration among the partners. Furthermore, new radio-architectures have been under analysis, development and measurements. A novel approach for detection of the in-plane vibrations has been found. Circuit simulation models for various elements, such as BAW line, piezo actuator and mechanical resonators, that can be implemented in the future MEMS radio, has been created. A MEMS-based reference oscillator has been designed to meet the strict GSM-specifications in the terms of phase-noise and power consumption. The properties of a MEMS delay line and RF MEMS filters have been theoretically studied and the theory has been verified in measurements with fabricated devices. In addition, a prototype of a MEMS-based millimetre wave phase shifter has been developed.

1 Partners and Funding

1.1 SMARAD Radio Laboratory, Helsinki University of Technology (RL)

The research group consists of subproject leader professor Antti Räisänen, senior researchers D.Sc.(Tech.) Sergey Dudorov, Ph.D. Dmitri Lioubtchenko, and D.Sc.(Tech.) Juha Mallat, and postgraduate students Lic.Sc.(Tech.) Dmitry Chicherin and M.Sc. Paavo Immonen (until 31 March 2005).

1.2 Circuit Theory Laboratory, Helsinki University of Technology (CT)

[1] SMARAD Radio Laboratory (RL), TKK, Otakaari 5A, FI-02150 Espoo
[2] Circuit Theory Laboratory (CT), TKK, Otakaari 5A, FI-02150 Espoo
[3] Micro and Nanosciences Laboratory (MNL), TKK, Tietotie 3, FI-02150 Espoo
[4] Optics and Molecular Materials (MPL), TKK, Tietotie 3, FI-02150 Espoo
[5] Sensors (VTT), VTT, Tietotie 3, FI-02150 Espoo

The research team consists of the subproject leader D.Sc.(Tech.) Timo Veijola and a postgraduate student Antti Kallio.

1.3 Micro and Nanosciences Laboratory, Helsinki University of Technology (MNL)

The research group consists of subproject leader professor Ilkka Tittonen and postgraduate students Mika Koskenvuori and Pekka Rantakari. The research group was initially part of the Metrology Research Institute, later part of the Laboratory of Optics and Molecular Materials and now part of the Micro and Nanosciences Laboratory.

1.4 Materials Physics Laboratory / Optics and Molecular Materials, Helsinki University of Technology (MPL)

The research team has included subproject leader Professor Matti Kaivola, senior researchers Saku Lehtonen, Tapani Makkonen and Jouni Knuuttila, and postgraduate students Olli Holmgren and Kimmo Kokkonen. In the beginning of the project, Professor Martti M. Salomaa acted as the subproject leader in the Materials Physics Laboratory (MPL) until his death in December 2004. In 2005 the activities of the microacoustic group of MPL were moved to the Laboratory of Optics and Molecular Materials.

1.5 Sensors, VTT

The research group consists of the subproject leader research professor Heikki Seppä, research professor Aarne Oja, senior researchers D.Sc.(Tech.), docent Tomi Mattila, Ph.D. Ville Kaajakari, and research scientist D.Sc.(Tech.) Ari Alastalo.

1.6 Funding

Table 1. Funding of the project in 1000 EUR in 2003-2006. Internal funding consists of manpower costs and operational expenditures provided by the organisation. The funding provided by the Academy of Finland and other external sources is also shown in the table.

Partner	Funding organisation	2003	2004	2005	2006	**Total**
TKK RL	TKK	30	45	45	40	**160**
	Academy	18	34	34	20	**106**
	Tekes	0	0	0	0	**0**
	Industry	0	0	0	0	**0**
TKK CT	TKK	8	12	12	8	**40**
	Academy	16	40	30	20	**106**
	Tekes	0	0	0	0	**0**
	Industry	0	0	0	0	**0**
TKK MNL	TKK	0	0	0	0	**0**
	Academy	18	34	34	20	**106**
	Tekes	0	0	0	0	**0**
	Industry	0	0	0	0	**0**
TKK MPL	TKK	8	18	6	6	**38**
	Academy	18	34	34	20	**106**
	Tekes	0	0	0	0	**0**
	Industry	26	57	39	13	**135**
VTT	VTT	40	80	80	0	**200**
	Academy	18	36	36	16	**106**
	Tekes	0	0	0	0	**0**
	Industry	0	0	0	0	**0**
Total		**200**	**390**	**350**	**165**	**1103**

2 Research Work

2.1 Objectives and Work Plan Restated from the Original Plan

The objective of the research project was to develop a novel highly integrated MEMS radio. This was planned to achieve by modeling, designing, manufacturing, and measuring prototypes of fundamental electroacoustic MEMS components and circuits consisting of these components. The work was organized into the following work packages.

Work packages

Analysis (CT, RL, MPL, MNL, VTT): Electroacoustic components will be investigated analytically and numerically (e.g., using FEM and APLAC®). Mechanical components include electroacoustic transducers, acoustic transmission lines, impedance transformers, filters, resonators, oscillators, mixers, frequency multipliers and directional couplers.

Equivalent-circuit modeling (CT, RL, MPL, MNL, VTT): Compact models will be derived and implemented as lumped or distributed electrical equivalent components in APLAC. APLAC enables simultaneous modelling of the mechanical and electrical parts of the circuits, as well as their interconnections, and will be utilized as the primary modelling platform. The existing APLAC MEMS component library will both be utilized and extended. On demand, measurement-based models will also be implemented.

Design of architectures and test devices (CT, RL, MPL, MNL, VTT): Novel microacoustical components will be designed for the well-established Silicon-On-Insulator (SOI) MEMS manufacturing process of VTT. Radio architectures suitable for MEMS implementation will be investigated. New architectures adapted to MEMS properties will be designed.

Manufacturing (MNL, VTT): Microacoustical SOI devices will be manufactured by VTT. This takes place free-of-charge to the MIRA project through collaboration with an internal strategic project “MEMS radio” of VTT launched in 2001. Using the manufactured MEMS components and CMOS circuits, a prototype of the radio architecture will be built. The goal is that the solutions selected enable high integration.

Measurements (RL, MPL, MNL, VTT): Test components and radio circuits will be measured both electrically and optically. The measurement results are used to test, improve and validate the component and circuit designs. Optical measurements are performed using the unique laser interferometer of the MPL. With optical probing of acoustic wave fields one can view the acoustic activity in micromechanical structures. The measured amplitude scans reveal mode structures and acoustic interactions such as intertrack couplings and waveguiding effects. The possibility to study and identify acoustic loss mechanisms is particularly interesting. Electrical measurements will be performed with the highest-quality equipment of VTT and TKK.

Intermediate goals

- Year 2003: prototypes of transducers, resonators and electroacoustic delay lines
- Year 2004: prototypes of filters, impedance transformers, mixers, multipliers, and matched transmission lines.
- Year 2005: Design and simulation of novel MEMS radio architectures
- Year 2006: Prototype of a novel MEMS radio

Researcher training

The objective in research training is to produce five Doctors of Technology by 2006. Each partner of the consortium produces one Doctor. In addition, the research teams contribute to the training of about ten young post-docs. There are professors and other experienced researchers in each group for the supervision of graduate students and young postdoctoral researchers. Fluent transfer of know-how and expertise between the partners is guaranteed through close collaboration and regular project meetings (once a month).

IPR issues

IPR issues are addressed in a consortium agreement to be signed before the start of the project. Patents are applied for new patentable innovations that are based on the results of the project.

2.2 Changes in the Objectives During the Work

The hardware prototype of a new MEMS based radio was left for future work. This was due to the unpredictably difficult component-level challenges that needed to be solved first during the project. On the other hand, the idea to study a MEMS-based high-impedance surface for beam steering came during the MIRA project, and this new research line was followed in RL during 2004 – 2006.

2.3 Final Report: Common Themes and Collaboration

Collaboration inside the MIRA consortium led to many useful advances in design, fabrication, analysis, and modelling of various MEMS-based components, because regular consortium meetings (in addition to frequent project meetings) gave an excellent forum for multidisciplinary discussions between specialists of different fields and of different aspects of MEMS. Therefore, all research carried out in this project gained from the existence of the MIRA consortium, not only the part described next.

The capacitive coupling usually used in MEMS components to transform an electric signal to mechanical motion and vice versa has a second-order force-voltage relation: $F \sim V^2$. This can be used to develop a mixer required in radio transceivers to transform the signal between a low-frequency base-band and a high-frequency RF band. Usually in MEMS mixers [WongMM],[vtt8] the resonance frequency of a capacitively-coupled micromechanical resonator is selected to be the mixer IF frequency. Such an arrangement utilizes the high quality factor of the MEMS for frequency selectivity such that no additional band-select filtering is needed. In theory it is also possible to parametrically amplify the IF signal by pumping the resonator at twice the IF frequency [vtt8]. However, to utilize MEMS in conventional mixer applications one faces great challenges. The quality factor need to be maximized and the coupling gap minimized in order to reach good conversion and reasonable impedance levels. High quality factor is beneficial to reduce the noise in the IF signal but it also makes the stability of the mixer against temperature variations a critical issue. Architecture development in the MIRA project started with a multicarrier MEMS radio architecture that utilizes a multiresonant spring-mass-chain delay-line [vtt7],[vtt8] as a mixer. During 2005 a simpler, more power efficient and highly integrable approach was identified that utilizes a two-carrier FSK modulation and uses a two-resonant MEMS plate structure for signal reception. A demonstrator based on this concept was designed.

Applicability of the scanning Michelson interferometer [mpl37] for the study of RF-MEMS components was first studied with the help of a hexagonal membrane resonator (f_{res}=1.1 MHz) featuring vibrations perpendicular to the sample surface. The sensitivity of the interferometer was clearly sufficient for detecting the membrane vibrations and several dozen different vibrations modes were discovered, each with a unique mode shape. However, many RF-MEMS components, such as the multiresonant spring-mass-chain delay-line [vtt7],[vtt8] mentioned above, feature vibrations parallel to the sample surface. Hence, measurements from the two-resonant MEMS plate structure were made to investigate whether the minute out-of-plane vibrations, resulting from the Poisson ratio of the silicon crystal, could be detected. Instead of clear coupling between the in-plane and out-of-plane vibrations, several parasitic out-of-plane vibrations were discovered masking the out-of-plane component resulting from Poisson ratio. However, during the measurements, a novel approach was developed for the direct detection of the in-plane vibrations and the two-resonant modes of the plate structure were directly imaged [mpl12], [mpl25]. Details of the technique are given in section 2.7. In 2005 – 2006 efforts were targeted at methods where interferometric measurement of the out-of-plane vibrations and the newly found vectorial measurement of the in-plane vibrations could be performed in vacuum. The need for such measurements is obvious as the majority of RF-MEMS components are to be operated under vacuum in order to achieve high quality factors, critical due to reasons given above, e.g., noise issues and stability. To facilitate such measurements a custom-built sample enclosure, 2cm x 1cm x 0.5cm metal case with a quartz window, and vibration isolated connections to vacuum pump was developed. Initial interferometric measurements of the mechanical vibrations in vacuum showed increase in amplitude and Q-value and a decrease in resonance frequency. These coincide with observations made in electrical measurements.

2.4 Final Report: SMARAD Radio Laboratory

Firstly, a feasibility study on RF-MEMS as a microwave filter was carried out during 2003-2004. This resulted in the Master's thesis [RL6] of Paavo Immonen in June 2004.

Secondly, applicability of a RF-MEMS mixer-filter for a multicarrier radio has been studied together with the VTT group. In a MEMS mixer-filter mixing is based on the nonlinear (second-order) force-voltage relation of capacitive transducers. Corresponding to each high-frequency carrier, there is a resonance in the mixer-filter at IF frequencies. An ideal mixer-filter down-converts the RF signals and also filters the resulting IF signals. Less noise is down-converted than with conventional band-pass filtering. No separate band-select filter is needed. However, the bandwidth of each IF signal is very narrow due to large Q-factors. Therefore, the data rate is low [RL8].

In 2004-2006 a MEMS-based high-impedance surfaces (HIS) have been developed for use as a low loss compact millimeter wave phase shifter [RL1]-[RL3],[RL7]. Such phase shifter can be developed by introducing a surface with variable impedance in, e.g., a rectangular metal or a dielectric rod waveguides. Placed along narrow walls of the rectangular metal waveguide or adjacent to the dielectric rod waveguide, the HIS affects the propagation constant, which results in changing the phase of the propagating wave [RL4]. Also the MEMS-based tunable HIS can be used as a reflector which does not need to obey the Snell's law [RL7], [RL9]. These new possibilities open new avenues for mm-wave steerable antennas, which are needed both in radar and in communications.

In an electronically tunable MEMS-based HIS, an array of MEMS capacitors, biased by an applied voltage and placed on a dielectric substrate with a ground plane, see Fig. 1, is used to provide tunability of the surface impedance.

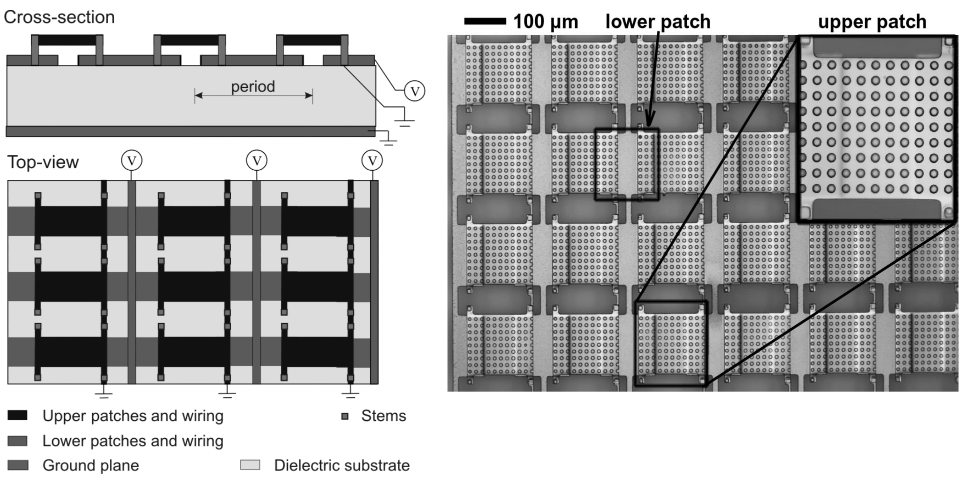


Fig. 1 MEMS-based tunable multi-layer HIS: design (left), and optical image (right)

The capacitive array is realized by two layers of metal patches shifted relative to each other: the lower patches are placed on the dielectric and the upper patches are fixed with four stems above the lower patches. If the period of the array of patches is much smaller than the wavelength of the field incident on the HIS or propagating above it, an effective surface impedance model can be used in order to characterize the electromagnetic behaviour of the structure. Surface impedance is related to effective resonant circuit parameters: capacitance C (determined by the period of the HIS and by the separation between the patches) and inductance L (proportional to the thickness of the dielectric layer). At the resonant frequency, $\omega_0 = \sqrt{1/(LC)}$, the effective surface impedance tends to imaginary infinity, and at the same time the phase of the electromagnetic wave reflection coefficient changes from ±180° to zero. The gap between the upper and lower patches is filled with air and controlled by an applied actuation voltage which decreases the gap and increases the MEMS capacitance. Consequently, both the effective surface impedance of the structure and its reflection phase change, for the frequencies close to the resonance of the structure.

We have already manufactured [RL5] two sets of MEMS-based HIS prototypes and demonstrated that the reflection phase changes by 282 degree over the measured frequency range (70 – 95 GHz), see Fig. 2, which will ensure large phase shift once the actuation voltage sources are connected to the MEMS capacitors. The resonance frequency of the structure is 82 GHz where the phase of the reflection coefficient is equal to zero degree. The losses at the resonant frequency are 5 dB, while the losses outside the resonance are about 2 dB. These losses can be explained by manufacturing nonidealities and a surface wave excited due to the opening between the sample and the waveguide.

The fabricated structure appeared to be too stiff to be actuated by reasonable values of the bias voltage. We foresee that longer term research work is needed to overcome the problems related to materials, fabrication, and modeling of such surfaces. Nevertheless, obtained results open large perspectives of using MEMS-based HIS for millimeter wave applications.

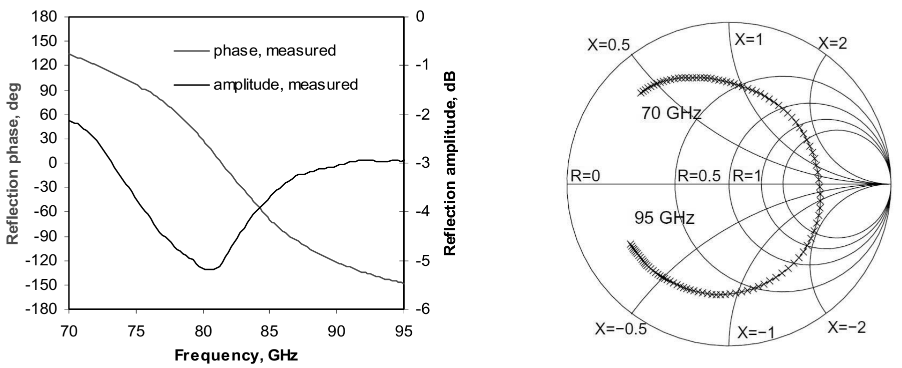


Fig. 2 Measured S_{11} characteristics of the tunable MEMS-based HIS: frequency dependence of the reflection phase and amplitude (left), and Smith chart (right)

In future, in the frame of the Nordite SARFA project, we will concentrate on decreasing losses of the structure and introducing voltage tuning of the MEMS capacitors in order to be able to control the surface impedance and obtain a low loss reconfigurable millimeter wave phase shifter based on a rectangular metal or a dielectric rod waveguide. We also are going to manufacture a larger surface with possibility to tune different rows of MEMS capacitors separately, which will allow us to create a gradient of the impedance throughout the surface and consequently the gradient of the reflection phase of the wave incident on it. Such a device can be used as an electronically reconfigurable beam steering antenna for millimeter wave automotive radar.

2.5 Final Report: Circuit Theory Laboratory

In 2003, circuit simulation model for a BAW line and for a simple model for piezo actuator were developed. The models were implemented in an external library file that is accessible for all partners of the consortium. Models for BAW resonators manufactured and measured by MNL were modelled, see Fig. 3.

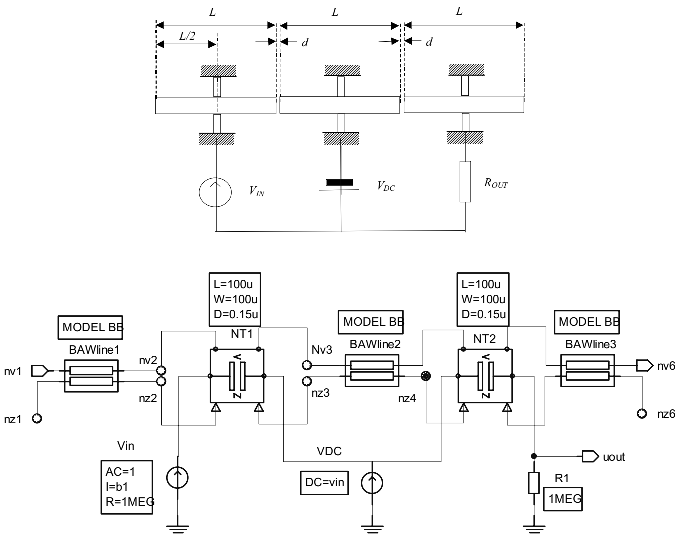


Fig. 3 Structure and measurement setup of a coupled BAW resonator manufactured and measured by MNL (above). Below is the equivalent circuit built of capacitive transducers in APLAC's MEMS library and the novel models for BAW lines.

In 2004, the development of a finite-difference model for a plate resonator started. Also, a model for a RBAR resonator, studied by MNL, was developed and implemented in the model library.

In 2005, an alternate modelling technique for the plate resonator was developed: a synthesis of reduced two port model. The method tuned out to be generally usable in compact modelling. The parameters for the synthesis can be derived directly from FEM simulations. A new method modelling transmission-line 2-ports was developed and published [CT1], see Fig 4.

In 2006, the finite-difference model was verified against FEM simulations. It turned out that the model could not predict the mechanical resonances with sufficient accuracy; the circuit was too complicated. Also, the initial plan to include piezoelectric characteristics to the model was impossible to complete. This is one of the reasons why the number of publications from Antti Kallio was less than originally planned. This delays his planned date of dissertation. Due to the financial reasons, Antti Kallio has moved to another project (TEKES/MASI/AMAZE), where his continues his research career. Here, it is worth of mentioning, that the results published in [CT1] could immediately be utilized in this new project in modelling a broadband transformer.

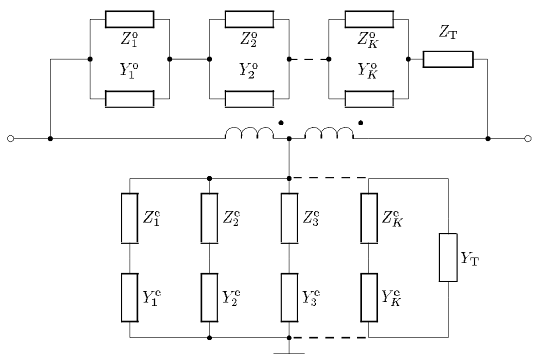


Fig. 4 Synthetized transmission line equivalent circuit [CT1].

Accurate FEM eigenvalue analysis of the measured (by MPL) square resonator was performed. The results were presented in the user meeting of the ELMER software [CT2]. Later, after this project, the knowledge in modelling RBAR resonators was utilized in modelling radial disk resonators [CT3, CT4].

2.6 Final Report: Optics and Molecular Materials / Micro and Nanosciences Laboratory

The first primary task was the finalization of a MEMS-based reference oscillator with custom-made integrated electronics. The core of the oscillator was a previously designed 2D-BAW resonator and the reference oscillator [mnl1] was designed to meet the strict GSM-specifications in the terms of phase-noise and to defeat the conventional quartz-oscillator in terms of power consumption.

Usually the silicon-based resonators with smallest feature sizes in the micrometer range possess mechanical resonances that are a few MHz. This is appropriate for example in oscillator-applications, but communication using transmission frequencies in the MHz-range requires the use of meter-size λ/4-antennae. To avoid the use of high impedance GHz-range resonators, the first logical task in a MEMS-based transceiver is to convert the signal from high communication frequency to the resonance frequency of the MEMS-device. Initially this was researched to be done with the aid of a local oscillator (LO) that is inside the transceiver [vtt8]. Another solution is to select the input signals so that non-linear processes convert the signal from the high communication frequency down to the eigenfrequency of the resonator [mnl1, mnl5].

In addition, the use of multi-resonant devices for simultaneous down-conversion and bit extraction in signal reception has been studied [mnl1] and it seems feasible to code the information in the phase of the mechanical vibration modes. New radio-architectures utilizing this feature have been under development and analysis with simulator tools.

2.7 Final Report: Materials Physics Laboratory / Optics and Molecular Materials

In 2003 the first laser interferometric measurements of an RF-MEMS membrane resonator fabricated by VTT were made. The results were promising and the sensitivity of the interferometer was found to be sufficient. Following that several other MEMS samples have been measured in the MIRA project. In 2004 a novel approach for detection of the in-plane vibrations was found. Here the etching-hole structure of the sample is utilized. The in-plane vibrations are imaged by measuring the intensity modulation of the laser beam reflected from the resonator chip at the edges of the release etch holes [mpl12, mpl25]. Combined with the high spatial resolution of the setup, a vectorial detection of the in-plane vibrations can be accomplished, see Fig. 5. In 2005 the in-plane detection was further developed to yield also the phase information of the vibrations. This improved technique was applied to analyse a MEMS delay line and MEMS double-ended tuning fork that can be used as a mixer. The results of these measurements are planned to be published in the near future. Furthermore, a vacuum system was designed and implemented to enable interferometric measurements in vacuum. Hence, we have been able to study mechanical Q-values of square-plate MEMS resonators in ambient air and in vacuum for both in-plane and out-of-plane vibration components [mpl28].

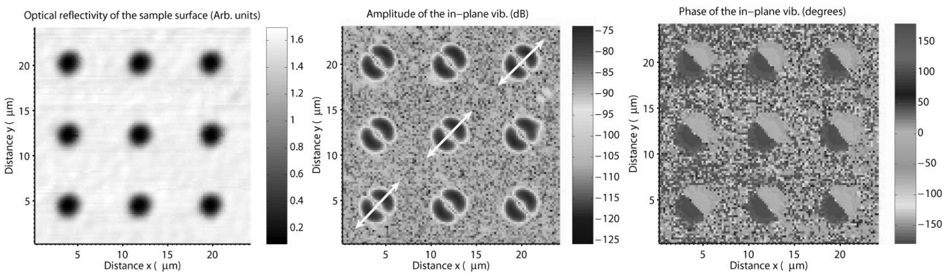


Fig. 5 Phase sensitive measurement of the in-plane vibrations in a square plate MEMS resonator: (left) optical reflectivity of the sample surface, i.e., a micrograph-like image, (middle) optical intensity modulation data yielding the relative amplitude of the in-plane vibrations, and (right) phase of the in-plane vibrations. The relative amplitude of the in-plane vibrations is obtained by locating the maximum value at each spot on top of the release-etch holes. The direction of the vibration is given by a line drawn through the maxima of the spot pair at each etch hole (white arrows in the figure). In this way, a displacement vector field of the in-plane vibration component is obtained.

Related to the MIRA project (though mainly funded through other sources), three D.Sc. theses have been completed during the MIRA project. Saku Lehtonen defended his D.Sc. thesis in November 2004. The work involved optimization of reflector and transducer structures, especially in connection with SAW ID tags. Such SAW tags can be thought of as simple passive micromechanical radios. They receive a radio signal via a small antenna and convert it to acoustic energy (surface acoustic wave) with the help of an interdigital transducer (IDT). The acoustic waves are then reflected from a series of acoustic reflectors and are transformed back into electrical signal by the IDT. Finally, the electrical signal is transmitted by the antenna. The number and location of the acoustic reflectors determines the code of the SAW tag. Tapani Makkonen completed his D.Sc. thesis entitled "Numerical Simulations of Microacoustic Resonators and Filters" in April 2005. His thesis involved modelling of radio frequency bandpass filters realized with thin-film bulk–acoustic wave resonators. Funding for this work was almost solely obtained from the industry. In June 2005, Jouni Knuuttila completed his D.Sc. thesis that dealt with the development of the laser-interferometer and its use for analysis of several SAW components.

2.8 Final Report: VTT

Nonlinearities are detrimental in filters that should be linear devices. Odd-order nonlinearities are especially unwanted as they can lead to interfering signals at the desired-user frequency f_0. For example, cubic mixing of two fundamental signals, having frequencies f_1 and f_2, results in third-order intermodulation (IM3) products at frequencies $2f_1 - f_2$ and $2f_2 - f_1$. If $f_1 = f_0 + \Delta f$ and $f_2 = f_0 + 2\Delta f$, the IM3 product at $2f_1 - f_2$ is at f_0 corrupting the desired-user signal at that frequency. This is illustrated in Fig. 6.

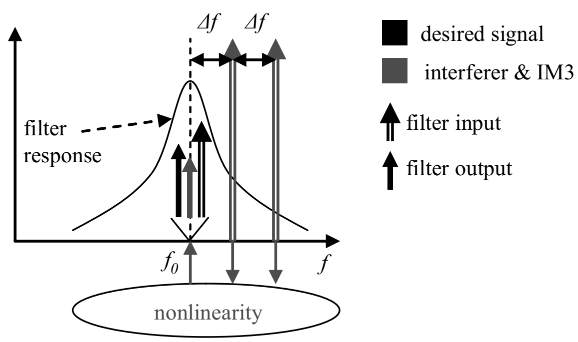


Fig. 6 A cubic nonlinearity generates IM products from the interfering signals at the desired-user frequency.

In the project, intermodulation properties of capacitively-coupled bandpass MEMS RF filters were analytically solved in closed form and the trade-off between linearity and insertion loss was quantified. The theoretical results were verified in circuit simulations as well as in measurements. The obtained formulas are more generally applicable than the results that have previously been published in literature [NguyenIM]. After the analysis, a systematic procedure to design MEMS filters was formulated. The conventional resistive 50Ω source and load termination was shown to typically result in a high insertion loss if good linearity is required with low-voltage operation. Consequently, it was found desirable to utilize the high resonator Q for voltage gain that is enabled by capacitive load termination at the filter output. This is possible in integrated receiver architectures, where 50Ω transmission lines are not needed between the antenna and the filter and between the filter and the LNA as shown in Fig. 7. With such an approach, MEMS filters could be used to construct a receiver front-end having a bank of narrow-band (ultimately channel-select) filters with different passbands to cover all the RX channels as suggested in [NguyenRX]

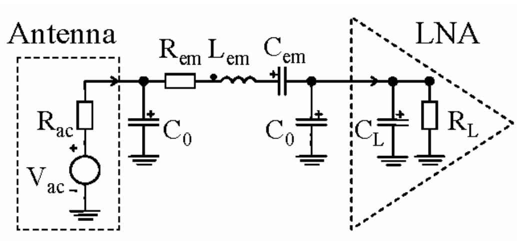


Fig. 7 First-order filter integrated with an antenna and an LNA.

Acoustic transmission lines have been utilized in several applications. For example, in wireless passive SAW RFID tags and sensors, the transmitted data is coded into a multitude of reflections of a SAW pulse that is generated (in response to a received radio pulse) and detected by an antenna connected to a SAW chip [ReindlSAW]. In these applications, long acoustic delays and short transmission distances guard against interference from multipath radio propagation.

In this project, usage of electrostatically-actuated longitudinal waves in a silicon rod for signal transmission was analyzed in detail and challenges due to high impedance levels were quantified. For HF frequencies, a MEMS resonator-chain structure with record low signal propagation was presented enabling miniaturization of time-delay components. The properties of the delay line were theoretically analyzed and the theory was verified in measurements with fabricated devices consisting of up to 80 series-connected MEMS resonators. The fabricated delay lines had still too high characteristic impedances for practical applications, but careful design can result in impedance levels of few kilo-ohms that can be acceptable in integrated solutions with properly-designed impedance transformers. In addition to a group velocity that is much lower than that for other acoustic delay lines (SAW or BAW), the MEMS line is characterized by a narrow-band response. This can be utilized in applications that would otherwise require a separate bandpass filter as in wireless transponder radios of sensors for which a possible structure is shown in Fig. 8. Compared to SAW devices, MEMS can dramatically reduce the size of the radio unit.

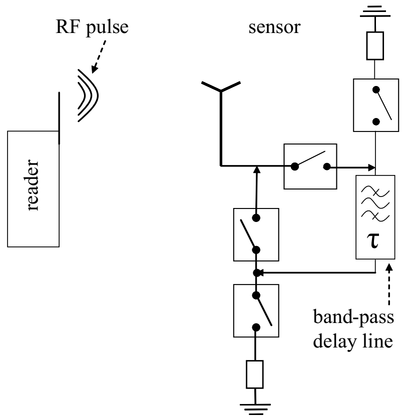


Fig. 8 Schematic of a simple delay-line transponder for low-power low-datarate communication in sensor applications.

3 International Aspects

VTT has developed novel low-power radios exploiting MEMS technology in the 6th framework IP-project MIMOSA (www.mimosa-fp6.com) in collaboration with EPFL, Micro Analog Systems, and CSEM. In this collaboration, VTT has focused in developing a monolithically integrated MEMS reference oscillator. VTT and Millilab (and through that also Radio Laboratory) are also members in the AMICOM NoE (Advanced microsystem for RF and millimeter wave communications, www.amicom.info) which collects leading European research institutes and universities in the field of RF MEMS. Radio Laboratory participates in ACE NoE (Antenna Centre of Excellence), which has interest in antennas utilizing MEMS. Furthermore, Radio Laboratory is the coordinator for METAMORPHOSE NoE (Metamaterials organized for radio, millimetre wave and photonic superlattice engineering), which has interest in MEMS-based artificial materials and surfaces. Radio Laboratory is continuing the research on MEMS-based HIS in a Nordite project SARFA together with KTH (Stockholm) and NTNU (Trondheim).

4 Publications and Academic Degrees

Table 2. Publications and academic degrees produced in the project. Numbers of different types of publications are given along with the reference numbers. List of refereed journal articles are given in Section 6.1, refereed conference papers in Section 6.2, monographs in Section 6.3 and theses in Section 6.4.

Partner	Type of publication	2003	2004	2005	2006	**Total**	Publication numbers
RL	Ref. journal art.				1	**1**	RL1
	Ref. conf. papers				4	**4**	RL2-5
	Monographs					**0**	
	Doctoral dissert.					**0**	
	Licentiate degrees			1		**1**	RL7
	Master degrees		1			**1**	RL6
CT	Ref. journal art.				1	**1**	CT1
	Ref. conf. papers					**0**	
	Monographs					**0**	
	Doctoral dissert.					**0**	
	Licentiate degrees					**0**	
	Master degrees					**0**	
MNL	Ref. journal art.				2	**2**	mnl1-2
	Ref. conf. papers		1	2	1	**4**	mln3-5
	Monographs						
	Doctoral dissert.						
	Licentiate degrees						
	Master degrees						
MPL	Ref. journal art.	3	6	3	4	**16**	mpl1-16
	Ref. conf. papers	5	6	2	3	**16**	mpl17-32
	Monographs					**0**	
	Doctoral dissert.		1	2		**3**	mpl33-35
	Licentiate degrees					**0**	
	Master degrees			1		**1**	mpl36
VTT	Ref. journal art.	1		1	4	**6**	vtt1-6
	Ref. conf. papers	1	1	1		**3**	vtt7-9
	Monographs					**0**	
	Doctoral dissert.				1	**1**	vtt10
	Licentiate degrees					**0**	
	Master degrees					**0**	

5 Other Activities

Every 3 months the MIRA consortium had a project meeting, where both progress and future plans were discussed. The MIRA project has its own homepages: http://www.ct.hut.fi/research/mira.html (password needed). APLAC-software has been made available to all project partners.

6 Publications

6.1 Refereed Journal Articles

[RL1] D. Chicherin, S. Dudorov, D. Lioubtchenko, V. Ovchinnikov, S. Tretyakov, and A.V. Räisänen, "MEMS-based high-impedance surfaces for millimetre and submillimetre wave applications," *Microwave and Optical Technology Letters*, vol. 48, no. 12, pp. 2570-2573, 2006.

[CT1] Antti Kallio, and Timo Veijola, "Synthesis of reduced equivalent circuits for transmission Lines", *IEEE Transactions on Circuits and Systems I* , vol. 53, pp 2255-2264, 2006.

[mln1] M. Koskenvuori and I. Tittonen, "GHz-range FSK-reception with microelectromechanical resonators", *Sensors and Actuators A*, submitted.

[mln2] M. Koskenvuori and I. Tittonen, "Towards GHz-range communication with micromechanical resonators: 2nd and 3rd nonlinear exitations", *Appl. Phys. Lett.*, submitted.

[mpl1] T. Makkonen, V.P. Plessky, W. Steichen, S. Chamaly, M. Solal, and M.M. Salomaa, "Fundamental mode 5 GHz surface-acoustic-wave filters using optical lithography," *Appl. Phys. Lett.*, vol. 83, no. 17, pp. 3596-3598, 2003.

[mpl2] S. Lehtonen, V.P. Plessky, J. Koskela, and M.M. Salomaa, "Second harmonic reflectors on 128° LiNbO3," *IEEE Trans. Ultrason., Ferroelect., Freq. Contr.*, vol. 50, no. 8, pp. 972-978, Aug. 2003.

[mpl3] S. Lehtonen, V.P. Plessky, C.S. Hartmann, and M.M. Salomaa, "Unidirectional SAW transducer for gigahertz frequencies," *IEEE Trans. Ultrason., Ferroelect., Freq. Contr.*, vol. 50, no. 11, pp. 1404-1406, Nov. 2003.

[mpl4] T. Makkonen, T. Pensala, J. Vartiainen, J. Knuuttila, J. Kaitila, and M.M. Salomaa "Estimating materials parameters in thin-film BAW resonators using measured dispersion curves," *IEEE Trans. Ultrason., Ferroelect., Freq. Contr.*, vol. 51, no. 1, pp. 42-51, Jan. 2004.

[mpl5] S. Lehtonen, V.P. Plessky, and M.M. Salomaa, "Short reflectors operating at the fundamental and second harmonics on 128° LiNbO3," *IEEE Trans. Ultrason., Ferroelect., Freq. Contr.*, vol. 51, no. 3, pp. 343-351, Mar. 2004.

[mpl6] J.V. Knuuttila, J.J. Vartiainen, J. Koskela, V.P. Plessky, C.S. Hartmann, and M.M. Salomaa, "Bulk-acoustic waves radiated from low-loss surface-acoustic-wave resonators," *Appl. Phys. Lett.*, vol. 84, no. 9, pp. 1579-1581, Mar. 2004.

[mpl7] S. Lehtonen, V.P. Plessky, N. Béreux, and M.M. Salomaa, "Minimum-loss short reflectors on 128° LiNbO3," *IEEE Trans. Ultrason., Ferroelect., Freq. Contr.*, vol. 51, no. 10, pp. 1203-1205, Oct. 2004.

[mpl8] S. Lehtonen, V.P. Plessky, N. Béreux, and M.M. Salomaa, "Phases of the SAW reflection and transmission coefficients for short reflectors on 128° LiNbO3," *IEEE Trans. Ultrason., Ferroelect., Freq. Contr.*, vol. 51, no. 12, pp. 1671-1682, Dec. 2004.

[mpl9] S. Lehtonen, V.P. Plessky, C.S. Hartmann, and M.M. Salomaa, "SPUDT filters for the 2.45 GHz ISM band," *IEEE Trans. Ultrason., Ferroelect., Freq. Contr.*, vol. 51, no. 12, pp. 1697-1703, Dec. 2004.

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[mpl16] O. Holmgren et al., "Analysis of a micromechanical resonator using scanning laser interferometer," *J. Micromech. Microeng.*, (to be submitted).

[vtt1] A.T. Alastalo, T. Mattila, and H. Seppä, "Analysis of a MEMS transmission line," *IEEE Trans. on Microwave Theory and Techniques*, vol. 51, no. 8, pp. 1977–1981, August 2003

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none

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PHOTONIC CRYSTAL BASED INTEGRATED OPTICS

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Abstract

The goal of this research project was to create a knowledge base and develop the infrastructure for fabrication of future optical devices based on photonic crystal structures. The two main lines of research followed in the project were the design, fabrication, and analysis of planar photonic crystal structures and the development and optimization of different schemes of white-light generation and other applications of microstructured optical fibers.

We have studied a novel photonic crystal geometry based on ring-shaped holes using plane-wave and time-domain methods. Larger bandgap, better in-plane confinement in cavities, higher sensitivity to refractive index variation are some of the interesting properties of such a structure. Fabrication of photonic crystals with ring-shaped holes in silicon-on-insulator was demonstrated. Besides, we have developed a method to characterize photonic crystal waveguides using multiple cavity resonances. Spin-on-glass was used to manufacture active slabs on glass. A photonic crystal etched into the slab is used to enhance photoluminescence.

We have studied the possibility of using a tapered microstructured fiber as mode-converter for efficient coupling of light to 2D photonic crystal waveguides. Simulations were carried out to determine the cross-section of the fiber to be employed. The study will serve as the first step to manufacturing of improved fiber-coupling devices for use with photonic crystal waveguides.

We have extensively studied supercontinuum generation in microstructured fiber when the optical nonlinearity in the fiber is pumped with mode-locked or Q-switched laser pulses. Several novel schemes have been developed of which one has been patented. We have also conducted an analysis along with simulations that demonstrate the feasibility of a microstructured fiber-based device to achieve optical switching, time-multiplexing and flip-flop operations. Also, we have demonstrated a novel switching concept based on a liquid-crystal-filled photonic crystal fiber placed transversally in between a conventional input and output fiber.

The scientific outcome of the project is 21 refereed journal articles, 17 refereed conference papers including 3 invited talks, 3 Master's theses, 2 Licentiate theses, 4+(2) Doctoral theses, 1 international patent application and contribution to the establishment of one spin-off company.

[1,2,4]Micro and Nanosciences Laboratory, Micronova, TKK, POB 3500, FI-02015 TKK
[1]Fiber-Optics Group, [2]Nanotechnology Group, [4]Micro and Quantum Systems Group
[3]VTT Microelectronics, Micronova, POB 1208, FI-02044 VTT
[5]Optics and Molecular Materials, Micronova, TKK, POB 3500, FI-02015 TKK

1 Partners and Funding

1.1 Fiber-Optics Group, TKK/Micronova [FOG/TKK]

The research group consists of subproject leader Docent Hanne Ludvigsen, postdoctoral researcher Goëry Genty, and postgraduate students Jesse Tuominen and Mikko Lehtonen.

1.2 Nanotechnology Group, TKK/Micronova [NTG/TKK]

The research group consists of subproject leader Professor Harri Lipsanen, postdoctoral researcher Mikael Mulot (50%), and postgraduate students Antti Säynätjoki and Karri Varis, and student Olli Sihvonen.

1.3 VTT Microelectronics, VTT/Micronova [MIC/VTT]

The research group consists of subproject leader research Professor Jouni Ahopelto, postdoctoral researcher Mikael Mulot (50%) and postgraduate student Sanna Arpiainen.

1.4 Micro and Quantum Systems Group, TKK/Micronova [MQS/TKK]

The research group consists of subproject leader Professor Ilkka Tittonen and postgraduate student Ossi Kimmelma and student Panu Ojala.

1.5 Optics and Molecular Materials, TKK/Micronova [OMM/TKK]

The research group consists of subproject leader Professor Matti Kaivola, senior researcher Scott C. Buchter and postgraduate student Esa Räikkönen.

1.3 Funding

Table 1. Funding of the project in 1000 EUR in 2003-2006. Internal funding consists of manpower costs and operational expenditures provided by the organisation. The funding provided by the Academy of Finland and other external sources is also shown in the table.

Partner	Funding organisation	2003	2004	2005	2006	**Total**
FOG/TKK	Academy	21	54	39	17	**131**
	Academy*	21	50	29	0	**100**
	TKK	10	35	35	10	**90**
	Industry	0	15	0	0	**15**
NTG/TKK	Academy	15	37	37	16	**105**
	TKK	21	35	30	15	**101**
MIC/VTT	Academy	12	43	37	13	**105**

	VTT	7	19	21	6	**53**
MQS/TKK	Academy	9	17	18	8	**52**
	TKK**	8	15	17	9	**49**
OMM/TKK	Academy	11	17	16	8	**52**
	TKK		28	17	10	**55**
	MOP-GS***			21	25	**46**
Total		**135**	**365**	**317**	**137**	**1004**

* Academy project: post-doctoral researcher
**Scholarship of 15000 EUR per year from TES for the period 1.7.2003-1.6.2005.
***Graduate School of Modern Optics and Photonics

2 Research Work

2.1 Objectives and Work Plan

WP1. Fabrication of 2D planar photonic crystals and integrated Microsystems

1.1 Design and fabrication of photonic crystal structures integrated with active elements such as lasers and LED’s based on III-V compound semiconductor material technology. Applications include higher efficiency light sources and elements for ultrafast all-optical switching. [NTG/TKK + MIC/VTT + MQS/TKK]

1.2 Characterization and subsequent optimization of the devices using conventional as well as advanced techniques such as scanning near-field optical microscopy (SNOM). [NTG/TKK + MIC/VTT + OMM/TKK + MQS/TKK]

WP2. Fiber-to-PC waveguide coupling

2.1 Design and fabrication of tapered photonic crystal fiber elements for efficient and compact coupling between planar photonic crystal devices and standard optical fiber. [FOG/TKK + OMM/TKK + NTG/TKK]

2.2 Characterization and optimization of the tapered fiber elements. [FOG/TKK]

WP3. Photonic crystal fiber components

3.1 Design and fabrication of compact supercontinuum sources based on photonic crystal fibers for optical coherence tomography and other applications requiring broadband light. [FOG/TKK + OMM/TKK]

3.2 Design and fabrication of new, compact switch devices using short sections of highly nonlinear photonic crystal fibers. [FOG/TKK + OMM/TKK]

3.3 Characterization and optimization of the switch devices. [FOG/TKK + OMM/TKK]

2.2 Final Report: Common Themes and Collaboration

The two main lines of research followed in the project have been the design, fabrication, and analysis of *planar photonic crystal structures* and the development and optimization of different schemes of white-light generation and other applications of *microstructured optical fibers.*

The planar photonic crystal part of the project was carried out in close collaboration between Partners 2, 3 & 4 and the photonic crystal fiber part by Partners 1 & 5. The conceptual similarity of the research problems made the regular consortium meetings fruitful opportunities for collaboration within the whole consortium. Furthermore, since summer 2004, all the partners have resided under one roof in Micronova, the joint micro- and nanotechnology centre of TKK and VTT. This clearly intensified the informal day-to-day contacts between the partners.

2.3 Final Report: Planar photonic crystal structures

Photonic crystals (PhCs) designed for near-infrared wavelengths are promising structures for future photonic circuits. Indeed, PhCs offer the possibility to confine, focus, guide or bend light efficiently in planar structures. Besides that, the small footprint of PhC-based devices is an essential asset for high density integration.

Development of planar photonic crystal fabrication methods

Fabrication of PhC waveguides has been developed at VTT. The main steps of the fabrication process are illustrated in Fig. 1. The limited size of the writing area in electron beam lithography limits the length of the PhC to about 100 μm. Therefore, the PhC waveguides must be coupled with conventional strip waveguides in order to be able to characterize their transmission properties (Fig 2a). Strip waveguides have been fabricated on commercial silicon-on-insulator (SOI) substrates. SOI is an attractive material platform for photonics because it can be processed using conventional microelectronics processing techniques and it allows for integration of electronic and photonic circuits on the same chip.

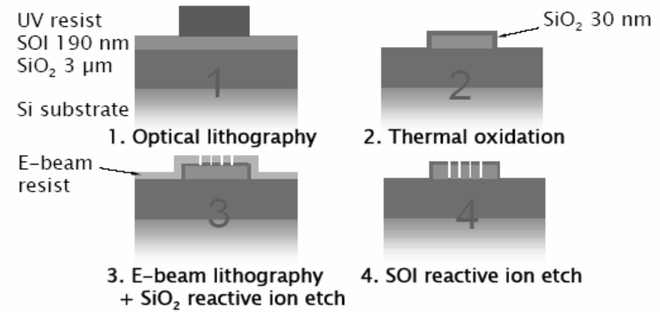


Fig. 1. Main steps of the fabrication process of a PhC waveguide.

PhC waveguides with three rows missing from the hexagonal air hole lattice (W3 waveguides) were patterned (Fig. 2a). The lattice constant *a* of the PhC lattice is equal to 460 nm. Details of the vertical layer structure are shown in Fig. 2b.

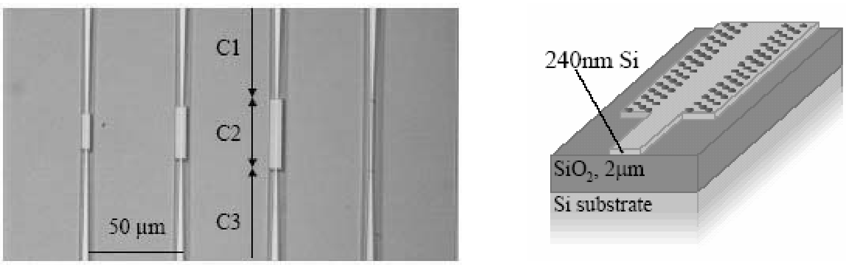


Fig. 2. a) Optical micrograph of W3 PhC waveguides inserted between conventional strip waveguides. A taper is necessary to bring the light from the 5...8 µm wide strip waveguides into the 1.2 µm wide PhC waveguides. The input waveguide, PhC waveguide and output waveguide are denoted with C1, C2 and C3, respectively. b) 3D schematic of the sample. Note that the Bragg mirrors described in the text are not drawn into this schematic illustration.

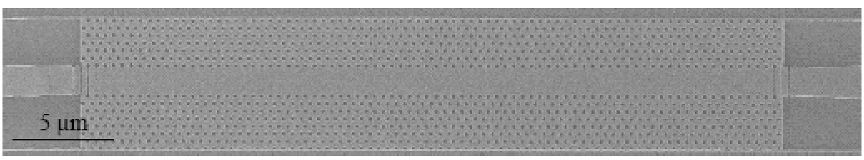
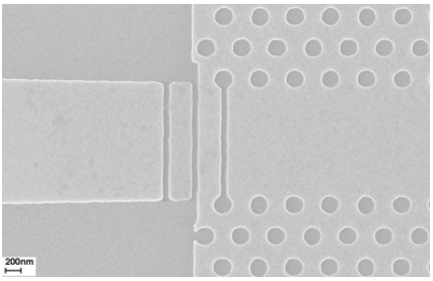


Fig. 3. Scanning electron micrograph of a fabricated PhC waveguide. The triple-groove Bragg mirrors at the waveguide ends define a Fabry-Pérot resonant cavity.

A Fabry-Pérot method for characterizing PhC waveguides

The PhC waveguides are usually patterned by e-beam lithography with a limited writing area (usually about 500 µm * 500 µm). In order to couple light into the PhC waveguide it needs to be patterned between two strip waveguides. The interface between the PhC waveguide and the strip waveguide introduces parasitic reflections that compromise the accuracy of transmission measurements. However, the Fabry-Pérot effect can be used in characterization of the PhC waveguide. We developed a method in which the reflections in the ends of the PhC waveguide are enhanced by patterning Bragg mirrors into the ends of the PhC waveguide and measuring transmission spectra of the sample (Fig. 4). With our method, the Fabry-Pérot effect in the strip waveguides is utilized as well.

a)



b)

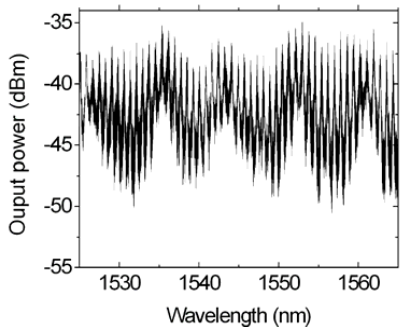


Fig. 4 a) End of a W3 PhC waveguide with a Bragg mirror in the PhC-strip waveguide interface, b) Transmission spectrum of such a sample.

The transmission spectra are a superposition of three sets of Fabry-Pérot fringes originating from resonances in the PhC waveguide, and in the input and output strip waveguides. However, when the strip waveguides are longer than the PhC waveguide, the Fabry-Pérot oscillations corresponding to those can be distinguished for having the shortest period. This makes it possible to treat the strip waveguides as wavelength dependent mirrors.

The measurements give a value of 16 dB/cm for the attenuation in the PhC waveguide, which means a loss of 3 dB for the waveguide with a length of 18.3 µm. This loss is shown as an 11 dB contrast between the maxima and minima values in the Fabry-Pérot fringe pattern. We also compared our method to the conventional Fabry-Pérot method, which is done by averaging out the oscillations in the strip waveguides. The Fabry-Pérot contrast was 7 dB over the waveguide length of 18.3 µm. Thus, our method showed a contrast enhancement of 4 dB.

Heterogeneous bonding

The development of photonics is limited by the lack of a universal optical material which can accomplish both active and passive functions with high efficiency and low cost. On the one hand, passive circuits are still dominated by silica and SOI. The SOI platform is all the more interesting that it is compatible with CMOS technology and can support integrated electronics. On the other hand III-V semiconductors remain the materials of choice for laser sources and detectors for telecommunication wavelengths. Therefore heterogeneous integration of III-V chips on top of silicon-based photonic circuits seems to be the most promising approach towards highly functional optical modules. In this work, we demonstrated fabrication of active PhC structures by combining

InP active devices and passive silicon based photonic crystal waveguides by chip bonding of InP onto silicon.

We used plasma bonding to manufacture silicon/InP hybrid waveguides. Such a waveguide would form the building block for integrated lasers or detectors in a silicon passive circuit. Contrarily to anodic bonding, plasma bonding is inexpensive and can be applied to small chips.

The bonded interface was inspected by ultrasound microscopy on test samples (Fig. 5). In spite of a few localized voids, the bonding quality is fairly good.

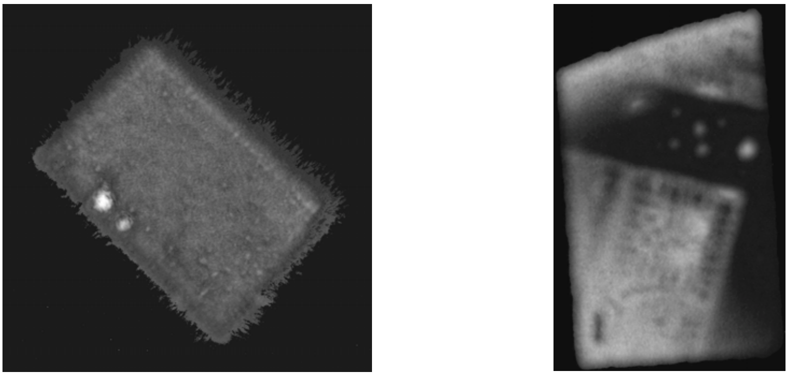


Fig. 5. Imaging of the bonding interface by ultrasound microscopy. Dark areas correspond to successful bonding (no reflection of ultrasound waves), whereas light areas are voids due to defects or surface patterns. The left image is for an InP sample bonded onto unpatterned silicon. The size of the sample is about 5 mm. On the right image, an InP chip is bonded on top of a silicon sample with a test pattern. The pattern is visible on the ultrasound micrograph.

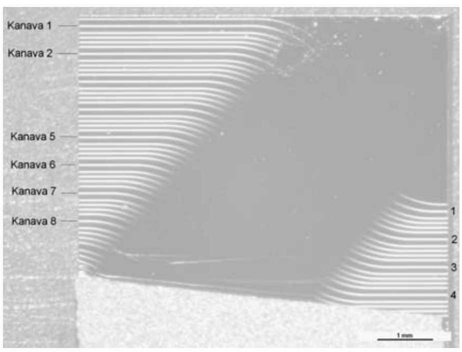


Fig. 6. Top view of the measured samples observed with an optical microscope. The InP sample can be seen at the bottom of the picture. Note that the input and output of the strip waveguide are not aligned so that a negligible part of scattered light at the input side is coupled into the collecting fiber at the output side.

Figure 6 shows a top view of the measured sample. The InP sample covers only a part of the silicon chip. The light intensity is low due to the poor coupling from the fiber into the waveguide. However, we measured a signal through most of the waveguides. We estimate that the InP chip induces an extra loss of 11 dB, mostly due to parasitic reflections at the interface between the strip waveguide and the hybrid waveguide.

Active photonic crystals

In this project, we have applied the concept of PhC to enhance the extraction efficiency of light from LEDs. In ordinary LEDs, the output power is limited by the fact that photons are trapped in the device by total internal reflection. A planar PhC patterned onto the LED surface can drastically improve the light extraction by coherent scattering in the periodic structure. We have studied the effect of a PhC on the emission from an active InP membrane bonded on top of glass. The membrane is on top of a 300 nm thick InGaAs layer. It contains four InGaAs quantum wells emitting at 1550 nm. A graphite lattice of holes has been etched through the membrane. The filling factor of the manufactured graphite lattice is relatively small (<30%) so that a large portion of the quantum wells is still intact (Fig. 8).

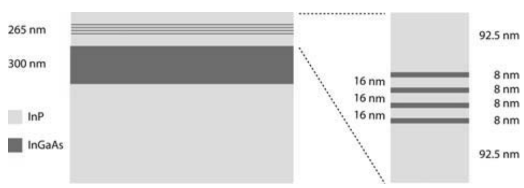


Fig. 7. Vertical structure of the MOVPE-grown InP sample.

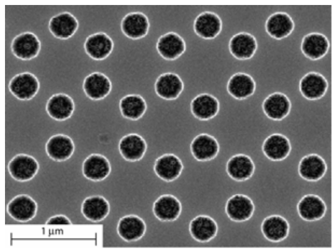


Fig. 8. PhC with graphite lattice etched into InP.

A critical step in the fabrication process was to develop a method to attach the membrane to the glass. Spin-on-glass bonding was applied. It is a flexible method compared to plasma bonding since it does not required ultra-smooth surface. Moreover, unlike other polymers used for bonding, spin-on-glass can stand temperatures as high as 300ºC. This is the temperature required for PECVD deposition of the SiN hard mask. Figure 9 shows a cut-view of the InP membrane sample obtained by scanning electron microscopy. The spin-on-glass bonding layer is between the PECVD and thermal oxide layers. The silicon substrate is visible below the thermal oxide layer.

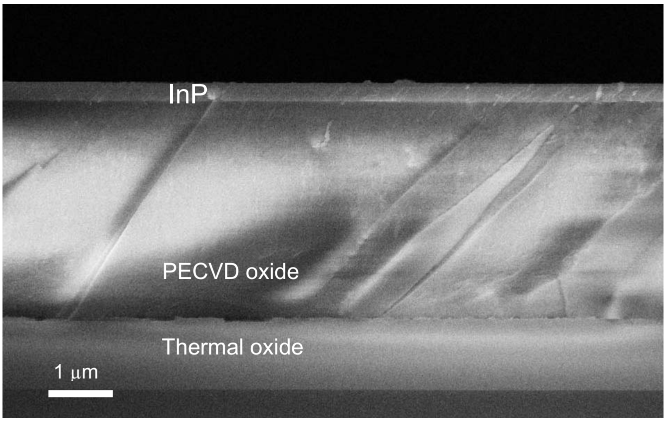


Fig. 9. Cut-view of the InP membrane by scanning electron microscope.

Photoluminescence measurement results are shown in Fig. 10. The sample was excited with a diode pumped solid-state laser emitting at 532 nm in the continuous wave regime. The PhC structure is found to amplify the photoluminescence signal at its best by a factor of nine over a wavelength range of 100 nm. The wavelength of the amplification peak is consistent with our simulations of the PhC band diagram. The wavelength range of the amplification spectrum can be shifted by tuning the lattice constant of the PC which is shown as different curves in the figure.

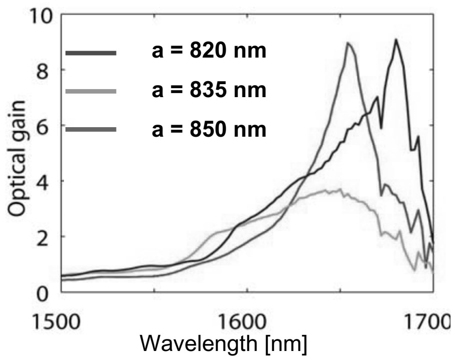


Fig. 10. Photoluminescence spectra of the active InP for three different PhC lattices. For all curves the excitation power is 60 mW (continuous wave regime).

PhCs with ring-shaped holes (RPhCs)

Photonic crystals are typically manufactured with round holes, because they are easy to pattern by electron beam lithography. However, other patterns may be more interesting for given applications. Photonic crystals with ring-shaped holes give more degrees of freedom to engineer the band structure. In this way, larger bandgaps can be achieved, which leads to PhC mirrors with higher reflectivity and resonant cavities with higher quality factor.

We observed that for the same air-fill factor, the bandgap in PhCs with ring-shaped holes is shifted to higher photon energies compared to conventional PhCs. This suggests that in PhCs with ring-shaped holes a larger portion of the light is propagating in the low index region. Therefore, one may expect a strong effect in the properties of these structures if the refractive index of the ambient is varied. This was tested by studying the transmission of a 1D cavity as a function of the ambient refractive index. The structure used in the FDTD simulations is described in Fig. 11. The 1D cavity is formed by two ΓM mirrors separated by a distance of 1.7*a* (*a* = lattice constant). The effective refractive index of silicon is 2.9 corresponding to a slab with a thickness of 240 nm. The structure is probed using a plane wave light source. The transmission spectrum of the structure in the wavelength range of the photonic gap exhibits a resonance peak. The quality factor is deduced from the width of the resonance peak. To analyze the sensitivity of the structure to variations of the refractive index, we measured the variation of the *Q*-factor when the refractive index in the rings is varied from 1.0 to 1.2.

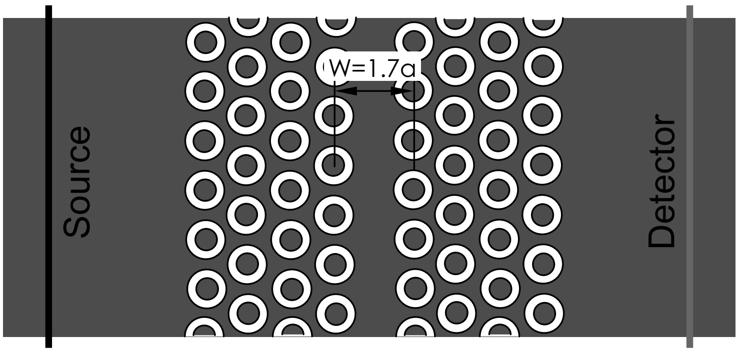


Fig. 11. Schematic of a 1D cavity with PhC with ring-shaped holes.

We used an air-fill factor of 25% for both the PhC with ring-shaped holes and the conventional PhC. For such a small air-fill factor we expect a larger reflectivity for the RPhC mirrors compared to the PhC mirrors (see Fig. 11). This explains why the RPhC cavity possesses a higher quality factor *Q* than the cavity made from a conventional PhC. More importantly, in the ambient refractive index range 1.0-1.2, the *Q*-factor of the RPhC cavity was found to be approximately twice as sensitive to refractive index variations as the cavity with round holes. The higher sensitivity together with the larger sidewall surface area of the RPhC structure makes the crystals with ring-shaped holes particularly interesting for sensing applications.

We chose the 1D cavity as an example, but other basic structures can be used to probe the ambient refractive index, such as point-defect cavities, and in-plane or out-of-plane PhC mirrors.

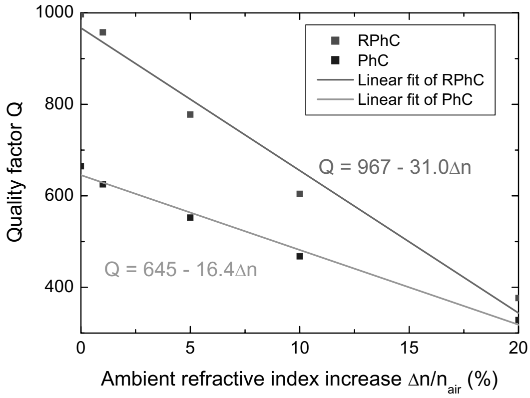


Fig. 12. Quality factor as a function of the refractive index increase inside the PhC holes. 1D cavities with PhC with ring-shaped holes and conventional PhC are compared. In both cases the air-fill factor is 25%. Linear fits show the average sensitivity over the range of refractive index variation.

Within this project, initial test runs to fabricate waveguide structures based on PhC with ring-shaped holes in SOI wafers have been completed. A result of such a structure is shown in Fig. 13.

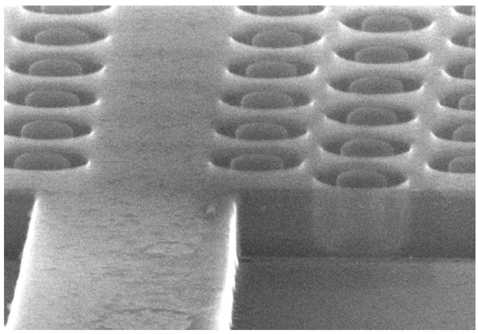


Fig. 13. Photonic crystals with ring-shaped holes.

Development of planar fabrication methods

Usual methods to produce planar integrated optical systems in a so-called MEMS process are optical lithography followed by various wet or dry etching processes.

At Micronova the most often used wafer material is SOI. Such systems that require release of some active, possibly even moving parts are made by HF sublimation etch of the intermediate oxide layer. In the beginning of this project this sublimation process step did not exist in the TKK process. Thus combining photonic structures with MEMS was in principle extremely demanding due to the problems in the accuracy of consecutive lithography steps and in the overall limitations of optical lithography.

In 2006, the TKK process was significantly developed. Major improvements took place in purchasing new equipment, two ALD reactors, new SEM/e-beam system and deep RIE etching station. The MQS Group at TKK developed a rather unique new process. Also the need for electron beam lithography for optics became easily realizable. The process combines the existing know-how of producing planar photonic crystal type components with a sequence that results in the final release of the whole MEMS components in the same process. This process starts by growing an alumina masking layer with ALD. Then the lithography is performed by direct writing by electric beam without any physical mask. This saves time and also reduces the costs of rather expensive lithography masks. Since the writing step is software based, the whole cad design is directly transferred to the e-beam. After DRIE all structures independent of the size become etched. The final step to possibly release some parts of the system is performed by optimized underetching. Thus the whole process can in principle be concluded in only 1-2 days. There are however, a number of limitations in using this process. All parts are written by e-beam which means that wafer level lithography is rather time consuming. Usually one can fabricate only very few components at a time, which, however, is quite suitable for fabricating prototypes. Large scale processing would require including nanoimprint techniques or even traditional HF etching. One more limitation is that the MEMS parts can only be actuated in the planar direction. However, in integrated optical systems, this should not be a severe drawback.

2.4 Final report: Photonic crystal fibers

Coupling light into photonic crystal waveguides

We have studied the possibility of using a tapered microstructured fiber as mode-converter for efficient coupling into 2D photonic crystal waveguides. Comprehensive simulations have been carried out to determine the cross-section of the fiber to be employed. Optimization of the taper profile to maintain single-mode propagation and obtain maximum coupling efficiency into the fundamental mode of the waveguide was also carried out. Our results show that the use of a tapered microstructured fiber can improve the coupling efficiency to the fundamental mode of a 2D photonic crystal waveguide by as much as 30% compared to standard solutions. In addition, the effect of various parameters such as ellipticity of the core of the tapered fiber and displacement between the tapered fiber and the waveguide were also investigated. The study performed in the course of this work will serve as the first step to manufacturing of fiber-coupling devices for use with photonic crystal waveguides [5,41,46].

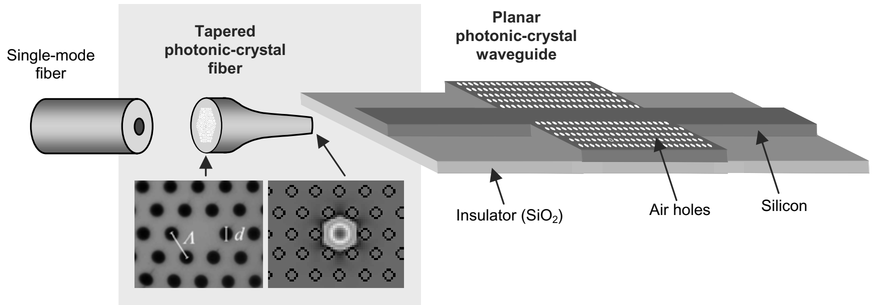


Fig. 14. Setup for coupling light into a waveguide using tapered microstructured fiber as the mode-field adapter.

Supercontinuum generation schemes

We have extensively studied supercontinuum (SC) generation in microstructured fiber when the optical nonlinearity in the fiber is pumped with short mode-locked or Q-switched laser pulses. Special attention was paid to extending the supercontinuum towards shorter wavelengths.

Nanosecond sources

We developed a compact nanosecond supercontinuum source that covers the spectral range from deep blue to infrared. This white-light source is based on a novel dual-wavelength pumping scheme that we have patented [51]. The pump source is a diode-pumped Q-switched and frequency-doubled Nd:YAG laser which puts out 2 ns long pulses. Dual-wavelength pumped SC generation was studied both theoretically and experimentally, and a good understanding of the underlying physical processes could be acquired. A set of fibers was designed and fabricated in order to decrease the short-wavelength cut-off of the SC. The main process contributing to continuum generation in the dual-wavelength scheme was found to be the cascaded cross-phase modulation induced by the infrared continuum on the visible pump wave [16]. Exploiting the same principle, we also constructed a compact SC source that uses a miniature Ti:Sapphire laser as pump [20]. The continuum generation of this source is initiated by four-wave mixing, after which cascaded cross-phase modulation extends the spectrum to visible wavelengths. The smooth spectrum of the source is shown in Fig. 16.

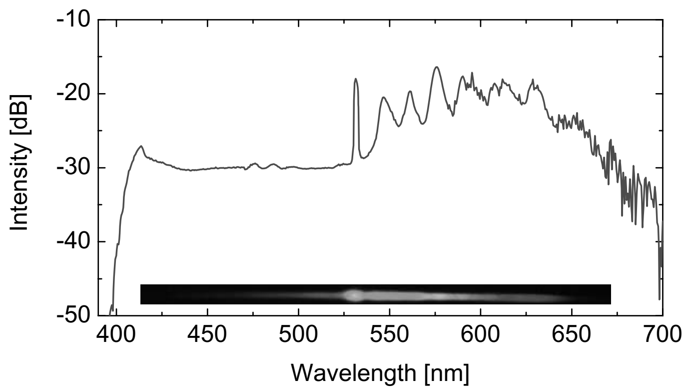


Fig. 15. Dual-wavelength pumped supercontinuum spectrum optimized for the blue region. Inset: Supercontinuum light dispersed using a grating.

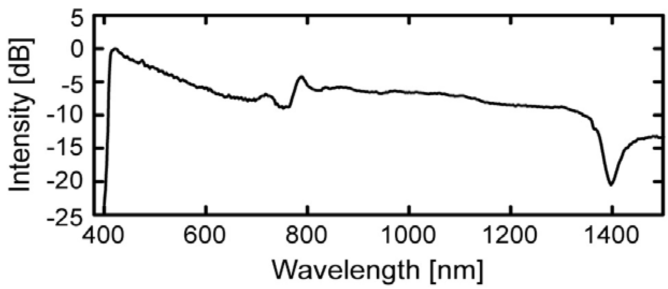


Fig. 16. Supercontinuum spectrum produced by using a miniature gain-switched Ti:Sapphire pump laser and a fiber optimized for generation of visible wavelengths [20].

A typical pump laser for a SC source is a passively Q-switched Nd:YAG laser that operates using the four-level transition of Neodymium at 1064 nm. However, 1064 nm is too long a wavelength to produce SC light that would cover the whole visible spectrum. Therefore, we have developed a high-peak power Nd:YAG laser that operates on the three-level transition of Neodymium at 946 nm. Unfortunately SC generation could not be demonstrated due to lack of fiber with suitable parameters. A schematic picture of the laser source that produces nanosecond pulses is presented in Fig 17.

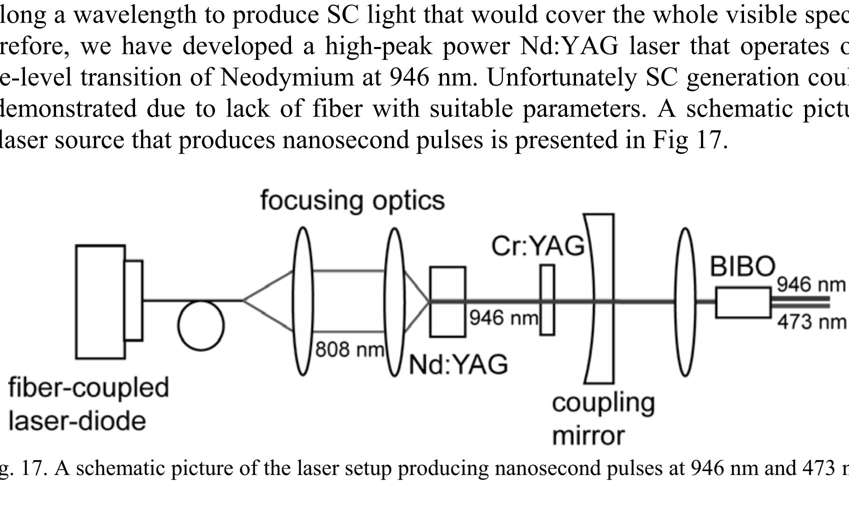


Fig. 17. A schematic picture of the laser setup producing nanosecond pulses at 946 nm and 473 nm.

Enhancement of the bandwidth of the supercontinuum generated in microstructured fibers with a tailored dispersion profile was demonstrated experimentally. The fibers are designed to have two zero-dispersion wavelengths separated by more than 700 nm, which results in an amplification of two dispersive waves at visible and infrared wavelengths. The underlying physics behind the broad continuum formation was analyzed in detail. The experimental observations were confirmed through numerical simulations [1,40,46]

We also investigated the effects of cross-phase modulation between the solitons and dispersive waves present in a supercontinuum generated in microstructured fibers by sub-30 fs pulses. Cross-phase modulation was again shown to have a crucial importance as it extends the supercontinuum towards the shorter wavelengths. The experimental observations were confirmed through numerical simulations [2,40,46].

In addition, we explored theoretically the possibility of generating broadband blue light by copropagating a short soliton pump pulse and a broader signal pulse in a microstructured fiber with the fiber zero-dispersion wavelength located between the center wavelengths of the pump and the signal pulses. We showed that the unique properties of microstructured fibers should allow for broadening of the signal pulse's spectrum by as much as a factor of 50 through the conjugate action of cross-phase modulation and soliton self-frequency shift. The physical mechanism that leads to this large spectral broadening was analyzed by solving an extended nonlinear Schrödinger equation [3,46]. Moreover, we proposed a setup for how to efficiently couple the pump and signal pulses into the microstructured fiber and how to tune their relative initial delay (see Fig. 18a). In order to obtain efficient broadening of the spectrum to both to the red and blue from the wavelength of the signal pulse, the dispersion profile of the the microstructured fiber should be such that the soliton first decelerates compared to the signal (inducing redshift), and subsequently accelerates due to soliton self-frequency shift (inducing blueshift) as is shown in Fig. 18b.

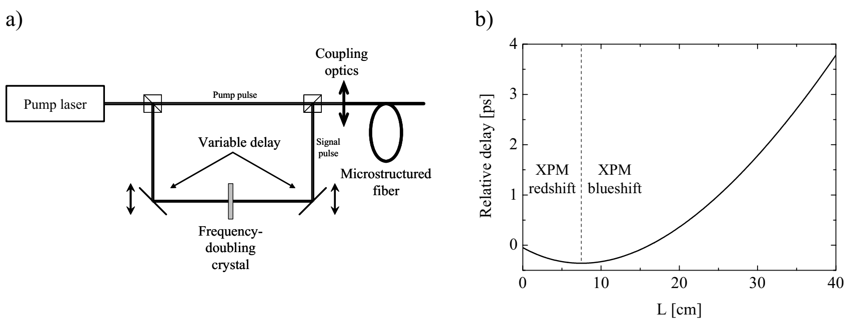


Fig. 18. a) Proposed setup for efficient broadband blue light generation. b) Relative delay of the pump and signal pulses for different values of fiber length. A positive value of the delay stands for signal trailing the pump.

Applications of supercontinua

A supercontinuum laser source is particularly useful in the context of spectroscopy as the broad bandwidth allows for characterization and identification of a wide variety of molecules through their absorption spectra. We performed experiments that show the benefit of supercontinuum light for probing the transmission properties of Erbium-doped fibers [4,46]. The technique allows for characterizing simultaneously the absorption bands of these fibers over a wavelength range that extends from the visible to the infrared. Furthermore, the compact supercontinuum source was also utilized to study the transmission of novel optical components such as photonic bandgap fibers and ultra-high reflectivity fiber-cavities.

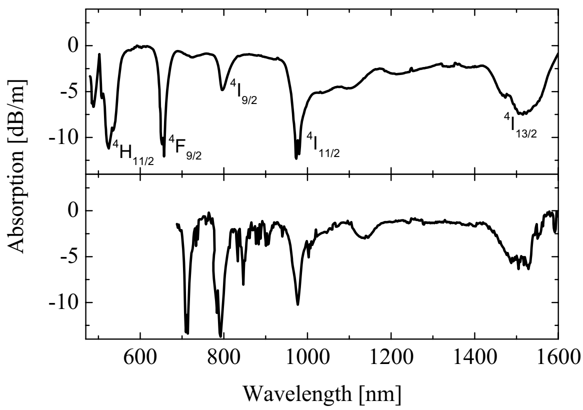


Fig. 19. Absorption spectra of Erbium-doped fiber sample measured using a supercontinuum generated with femtosecond (upper curve) and nanosecond (lower curve) pump pulses.

Light switches

All-optical switches and add-drop (de)multiplexers constitute some of the fiber-based components highly desirable in all-optical communication systems. For this purpose, microstructured fibers offer great potential as their enhanced nonlinearity can be conveniently used to realize logic functions. We conducted an extensive analysis along with simulations that demonstrate the feasibility of a microstructured fiber-based device to achieve optical switching, time-multiplexing and flip-flop operations [6,46]. The operation principle relies on the bistable behavior of a ring-resonator that includes a microstructured fiber as the nonlinear medium. The response of the device as a function of bit-rate and duty cycle was characterized, showing processing rates up to several MHz.

By filling the air-holes of photonic crystal fiber with a material whose optical properties are sensitive to external influences such as electric or magnetic fields or temperature, the guiding properties of the fiber can be varied. We have explored the possibility of realizing a photonic crystal based all-optical switch by introducing active materials such as polymers or liquid crystals into the holes of the fiber. In this work, we made use of our experience with applying gas-filled photonic bandgap fibers as effective gas sensors. We demonstrated a novel switching concept based on a liquid-crystal filled photonic crystal fiber that was placed transversally in between a conventional input and output fiber [18,48]. This switch-concept does not need any additional optical components such as couplers or filters, because the control beam is not guided along the same path as the signal light as is the case for many other designs. Fiber samples made from lead silicate and silica were studied. A continuous operating range from 600 to 1700 nm was achieved with an extinction ratio of 30 dB and insertion losses of ~3 dB for the lead silicate fiber. Furthermore, by designing the liquid-filled fiber to have a photonic band-gap for only one polarization could result in a single polarization device.

a) b)

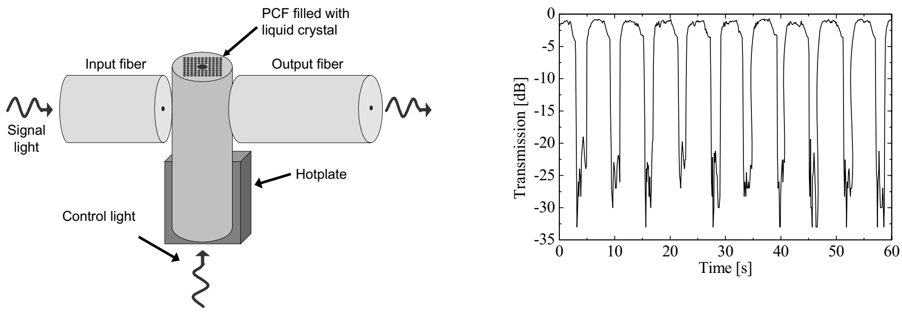


Fig. 20. a) Fiber-optic switch based on liquid-crystal-filled hollow-core microstructured fiber. b) The transmission is modified by controlling the orientation of the liquid-crystal molecules and thus the polarization rotation along the fiber by an external optical field.

3 International Aspects

The Fiber-Optics Group (FOG/TKK) is an active partner in the COST Action P11 "Physics of linear, nonlinear and active photonic crystals". H. Ludvigsen acts as Finland's representative in this action.

Several presentations, including invited talks, have been given at international conferences by the consortium members [22-39]. FOG/TKK organized a two-day workshop on photonic crystal fibers in December in Micronova. In the period 12-21 December 2004, Prof. R. Buczynski from Warsaw University in Poland visited Micronova for a short term scientific mission (STSM/COST) [29].

The commercial version of our patented supercontinuum source was in February 2005 awarded an international Photonics Circle of Excellence Award, which is annually given to the top 25 most innovative photonics products.

VTT/MIC is partner in a European Union IST Programme "Photonic Hybrid Architectures based on two- and three-dimensional Silicon Photonic Crystals, PHAT". The scientific innovations and technological knowledge obtained in this TULE program have provided a valuable contribution to the PHAT Program. In addition, MIC is partner in PHOREMOST, which is a Network of Excellence in nanophotonics in FP6.

4 Publications and Academic Degrees

Table 3. Publications and academic degrees produced in the project.

Partner	Type of publication	2003	2004	2005	2006	**Total**	Publication numbers
FOG/TKK	Ref. journal art.	-	2	6	3	**11**	1-8,14,17,18
	Ref. conf. papers	-	4	4	2	**10**	22-25,27-29,32,33,36
	Monographs	-	-	-	-	**0**	
	Doctoral dissert.	-	1	1	1	**3**	40,46,48
	Licentiate degrees	-	1	-	-	**1**	41
	Master degrees	-	-	-	-	**0**	
NTG/TKK	Ref. journal art.	1	1	3	2	**7**	9-13,15,21
	Ref. conf. papers	-	1	2	3	**6**	26,30,31,39
	Monographs	-	-	-	-	**0**	
	Doctoral dissert.	-	-	1	-	**1**	44
	Licentiate degrees	-	-	-	-	**0**	
	Master degrees	-	-	-	1	**1**	47
MIC/VTT	Ref. journal art.	-	-	1	2	**3**	11,15,21
	Ref. conf. papers	-	1	2	2	**5**	26,30,31,37,38
	Monographs	-	-	-	-	**0**	
	Doctoral dissert.	-	-	-	-	**0**	
	Licentiate degrees	-	-	-	-	**0**	
	Master degrees	-	-	-	-	**0**	
MQS/TKK	Ref. journal art.	-	-	-	1	**1**	19
	Ref. conf. papers	-	-	-	1	**1**	34
	Monographs	-	-	-	-	**0**	
	Doctoral dissert.	-	-	-	-	**0**	
	Licentiate degrees	-	-	1	-	**1**	45
	Master degrees	-	1	-	-	**1**	42
OMM/TKK	Ref. journal art.	-	1	-	4	**5**	1,14,16,19,20
	Ref. conf. papers	-	3	-	2	**5**	22,23,25,34,35
	Monographs	-	-	-	-	**0**	

Doctoral dissert.	-	-	-	-	**0**	
Licentiate degrees	-	-	-	-	**0**	
Master degrees	-	1	-	-	**1**	43

5 Other Activities

The kick-off meeting of this consortium was held on 3 September 2003. Since then the consortium has met eight times where each participant has given a 10-minutes presentation on her or his achievements. The partners FOG/TKK, MQS/TKK, and OMM/TKK moved in summer 2004 to Micronova so that all the partners of the consortium are now under the same roof. This has clearly increased the efficiency of the collaboration between the different partners and contributed to making Micronova one of the leading centers of photonics research in Finland. Furthermore, the project has contributed to the establishment of one spin-off company (Arctic Photonics, www.arcticphotonics.com).

Several presentations, including a plenary [57] and an invited [60] talk, have been given at national conferences. In addition, the project has had popular exposure on the following forums:

1. TKK NYT, 18 June 2004
2. Tiedotorstai, 3 March 2005, Department of Electrical and Communications Engineering, Helsinki University of Technology
3. Tekniikka&Talous, 14 April 2005
4. Polysteekki, May 2/2005.

6 Publications

6.1 Refereed Journal Articles

[1] G. Genty, M. Lehtonen, T.P. Hansen, M. Kaivola, and H. Ludvigsen, “Enhancement of supercontinuum generated in microstructured fiber”, Opt. Express **12** (2004) 3471-3480.

[2] G. Genty, M. Lehtonen, and H. Ludvigsen, “Effect of cross-phase modulation on supercontinuum generated in microstructured fibers with sub-30fs pulses”, Opt. Express **12** (2004) 929-934.

[3] G. Genty, M. Lehtonen, and H. Ludvigsen, “Route to broadband blue light generation in microstructured fibers”, Opt. Lett. **30** (2005) 756-758.

[4] M. Lehtonen, G. Genty, and H. Ludvigsen, “Absorption and transmission spectral measurements of fiber-optic components using supercontinuum radiation”, Appl. Phys. B **81** (2005) 231-234.

[5] M. Lehtonen, G. Genty, and H. Ludvigsen, “Tapered microstructured fibers for efficient coupling to optical waveguides: a numerical study”, Appl. Phys. B **81** (2005) 295-300.

[6] G. Genty, M. Lehtonen, and H. Ludvigsen, “Optical bistability in a high-finesse nonlinear microstructured fiber cavity”, Appl. Phys. **B** 81 (2005) 357-362.

[7] G. Genty, T. Ritari, and H. Ludvigsen, “Supercontinuum generated in large mode-area microstructured fibers”, Opt. Express **13** (2005) 8625-8633.

[8] H. Ludvigsen, “Novel devices based on photonic crystal fibers”, in SPIE **5950** (2005) 59500S-1 - 59500S-7.

[9] K. Varis and A.R. Baghai-Wadji, "Pseudo-spectral analysis of radially-diagonalized Maxwell's equations in cylindrical co-ordinates", Opt. Express **11** (2003) 3048-3062.
[10] K. Varis and A. R. Baghai-Wadji, "A novel 3D pseudo-spectral analysis photonic crystal slabs", ACES Journal **19** (2004) 101-111.
[11] K. Varis, M. Mattila, S. Arpiainen, J. Ahopelto, F. Jonsson, C. M. Sotomayor Torres, M. Egen, and R. Zentel, "Reflection of focused beams from opal photonic crystals", Opt. Express **13** (2005) 2653-2667.
[12] A. Huttunen, K. Varis, K. Kataja, J. Alkio, and P. Törmä, "Guiding and reflecting light by boundary material", Opt. Commun. **244** (2005) 147-152.
[13] K. Varis and A. R. Baghai-Wadji, "A 2D pseudo-spectral approach of photonic crystal slabs", ACES Journal **20** (2005) 107-118.
[14] E, Räikkönen, G. Genty, O. Kimmelma, M. Kaivola, K. P. Hansen, and S.C. Buchter, "Supercontinuum generation by nanosecond dual-wavelength pumping in microstructures optical fiber", Opt. Express **14** (2006) 7914-7923.
[15] A. Säynätjoki, M. Mulot, S. Arpiainen, J. Ahopelto, and H. Lipsanen, "Characterization of photonic crystal waveguides using Fabry–Perot resonances", J. Opt. A: Pure Appl. Opt. **8** No 7 (2006) S502-S506.
[16] E. Räikkönen, M. Kaivola, and S.C. Buchter, "Compact supercontinuum source for the visible using gain-switched Ti:Sapphire laser as pump", JEOS Rapid Communications **1** (2006) 06012.
[17] J. Dudley, G. Genty, and S. Coen, "Supercontinuum generation in photonic crystal fibers", Reviews of Modern Physics **78**, (2006) 1135-1189.
[18] J. Tuominen, H. Hoffrén, and H. Ludvigsen, "All-optical switch based on liquid-crystal infiltrated photonic bandgap fiber using transverse geometry", Appl. Phys. Lett. (submitted 2006).
[19] O. Kimmelma, I. Tittonen, M. Kaivola, and S.C. Buchter, "Short pulse, high peak power, diode pumped, passively Q-switched 946 nm Nd:YAG laser", Opt. Commun. (submitted 2006).
[20] E. Räikkönen, M. Kaivola, and S.C. Buchter, "Observation of broadband nondegenerate pump four-wave mixing in microstructured optical fiber", to be submitted (2006).
[21] A. Säynätjoki, M. Mulot, S. Arpiainen, J. Ahopelto, and H. Lipsanen, "Photonic crystals with ring-shaped holes", to be submitted (2006).

6.2 Refereed Conference Papers

[22] S.C. Buchter, M. Kaivola, and H. Ludvigsen, "Compact, spectrally smooth, nanosecond infrared continuum source with 700 nm bandwidth", Proc. Optical Fiber Communication Conference (OFC 04), in Los Angeles, California, US, paper ThA7 (talk).
[23] S.C. Buchter, M. Kaivola, and H. Ludvigsen, "Miniature supercontinuum laser sources", Proc. Conference on Laser and Electro-Optics (CLEO/IQEC 04), in San Francisco, US, paper CTuP58.
[24] T. Ritari, J. Tuominen, J.C. Petersen, and H. Ludvigsen, "Photonic bandgab fibers: Optical properties and device applications", Proc. Conference on Information Technology and Communication (ITCom 2004), in Philadelphia, US, paper 5596-33 (invited talk).
[25] S.C. Buchter, B. Andersen, M.D. Nielsen, K.P. Hansen, and H. Simonsen, "Nanosecond supercontinuum generation at the mJ level", SPIE European Symposium on Optics and Photonics in Security and Defence (25-28 October 2004, London, UK).
[26] A. Säynätjoki, S. Arpiainen, J. Ahopelto, and H. Lipsanen, "High-index-contrast optical waveguides on silicon", Proc. International Conference on Physics of Semiconductors, Flagstaff, USA, 2004, p. 1537.
[27] H. Ludvigsen, "Novel supercontinuum sources", Proc. 6th International Conference on Transparent Optical Networks/3rd European Symposium on Photonic Crystals (ICTON/ESPC 2005), in Barcelona, Spain, paper Mo.A.4. (invited talk).
[28] H. Ludvigsen, "Novel devices based on photonic crystal fibers", Proc. SPIE Europe, in Warsaw, Poland, 2005 paper [5950-29] S7 (invited talk).
[29] R. Buczynski, D. Pysz, T. Ritari, P. Szarniak. W. Saj, I. Kujawa, H. Ludvigsen, and R. Stepien, "Hollow-core photonic crystal fiber with square lattice", Proc. SPIE Europe, in Warsaw, Poland, 2005, paper [5950-42] S9 (talk).
[30] M. Mulot, A. Säynätjoki, S. Arpiainen, H. Lipsanen, and J. Ahopelto, "Photonic crystal slabs with ring-shaped holes in a triangular lattice", Proc. 6th International Conference on Transparent Optical

Networks/3rd European Symposium on Photonic Crystals (ICTON/ESPC 2005), Barcelona, Spain, 2005, paper Mo.C2.7 (talk).
[31] A. Säynätjoki, M. Mulot, S. Arpiainen, H. Lipsanen, and J. Ahopelto, “Characterization of photonic crystal waveguides using Fabry-Pérot resonances”, Proc. Optical Microsystems (OμS'05), Capri Island, Italy, 15-18 September 2005, paper 3 (talk).
[32] G. Genty, T. Ritari, and H. Ludvigsen, “Supercontinuum generation in large mode-area microstructured fibers”, Proc. 31st European Conference on Optical Communication (ECOC 2005), in Glasgow, Scotland, 2005 paper We4.P.6.
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6.3 Monographs

None

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ULTRA-FAST MICROLASER MODULE FOR OPTICAL COMMUNICATIONS

Harri Lipsanen[1]

Abstract

The project is based on a collaboration between professor Harri Lipsanen from Optoelectronics Laboratory (presently Micro and Nanosciences Laboratory), Helsinki University of Technology and professor Seppo Honkanen and professor Axel Schultzgen from College of Optical Sciences, University of Arizona. An ultrafast optical pulse generator based on an erbium:glass waveguide laser with a GaInNAs/GaAs saturable absorber mirror has been studied.

A wide mapping of optimal basic growth parameters for dilute nitride materials and development of GaInNAs quantum well structures has been carried out. By combining the GaInNAs quantum wells and the AlAs/GaAs Bragg mirror, a semiconductor saturable absorber structure operating at 1050 nm was first fabricated. The effect of nitrogen content on the recombination time of the quantum wells will be used to develop even faster mode locking of the waveguide laser as the operating wavelength of the SESAM will also be modified towards longer wavelengths and finally to 1.55 μm. Low birefringence in buried silver-sodium-ion exchanged glass waveguides has been demonstrated. Birefringence on the order of 10^{-6} for waveguide mask opening widths ranging from 2 to 10 μm can be obtained by post processing the sample through annealing at an elevated temperature. This unique feature of ion-exchanged waveguides may be of significant importance in a wide variety of integrated photonic circuits requiring polarization independent operation. Moreover, lasing operation in 1-cm long waveguide cavities on phosphate glass doped with varying concentrations of erbium and ytterbium has been shown. Waveguides fabricated by silver film ion exchange process typically feature a propagation loss below 0.15 dB/cm and a good mode matching with a fiber. The measured small-signal gain was approximately 4 dB/cm at signal wavelength (1535 nm). The measured output power of the laser was above 18 mW.

The project has generated 25 refereed journal articles, 13 refereed conference papers, a master's thesis and 1 doctoral thesis (3 more in preparation).

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1 Partners and Funding

1.1 Micro and Nanosciences Laboratory (MNS), Helsinki University of Technology

The research group consists of project leader professor Harri Lipsanen, post-doc Teppo Hakkarainen and graduate students Outi Reentilä, Sanna Yliniemi and Marco Mattila. Moreover, Sanna Yliniemi has worked both in the Optical Sciences Center, University of Arizona and in MNS of TKK. Graduate students Lauri Knuuttila, Aapo Lankinen and Tapio Rangel-Kuoppa have worked partially in the project.

1.2 Optical Sciences Center (OSC), Arizona, USA (not funded by the Academy)

The research group is led by professor Seppo Honkanen. Sanna Yliniemi worked over two years in his group. They have close collaboration with professor Jacques Albert, Carleton University, Ontario, Canada.

1.3 Funding

Table 1. Funding of the project in 1000 EUR in 2003-2006. Internal funding consists of manpower costs and operational expenditures provided by the organisation. The funding provided by the Academy of Finland and other external sources is also shown in the table.

Partner	Funding organisation	2003	2004	2005	2006	**Total**
MNS/TKK	TKK	32	57	60	30	**177**
	Academy	50	100	100	50	**300**
	Industry	0	0	0	0	**0**

2 Research Work

2.1 Objectives and Work Plan (from research plan)

The material studies will include the design and growth of the epitaxial structures and their optical characterization. The design of the epitaxial structures will be done in cooperation with OSC and the growth at OEL (now MNS) using a new, state-of-the-art Thomas Swan MOVPE equipment. The structural characterization will be performed at OEL. The optical characterization of the saturable absorber structures will be performed at OSC using a premium femtosecond laser facility. These extensive materials studies will be complemented by having the use of a glass waveguide laser test-bed to characterize the fabricated semiconductor saturable absorber mirrors. The Er-doped waveguide amplifiers developed at OSC are ideal for the potential application due the large intracavity gain and small mode-size, which are key requirements for the gain medium of a mode-locked laser with ultra-high repetition rate. The waveguide experiments together with the measurements of the materials' nonlinear absorption dynamics provide the essential feedback for material design and growth optimization.

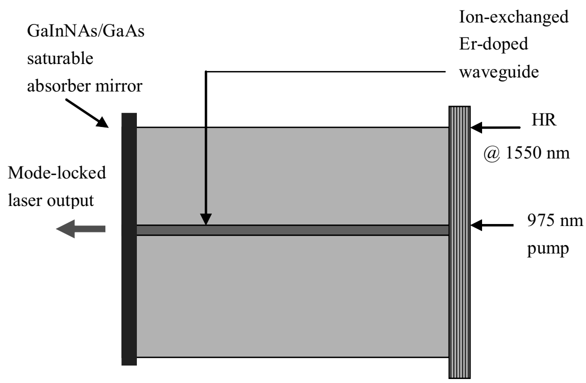

Fig. 1. Schematics of a compact 40-GHz mode-locked Er:glass waveguide laser..

The saturable mirror can be fabricated entirely of semiconductor layers with a total thickness of only a few microns. The short length makes it possible to directly butt the mirror against the gain medium (the Er-doped waveguide in this program) to form one end of the cavity. The laser can be very compact because no additional optical elements are required to couple light into the nonlinear mirror. The compact size also means that mode locking can be achieved with ultra-high repetition rates. An optically nonlinear mirror is a passive device, so there is no need for the separate drive electronics that are used with actively pulsed lasers

Task 1: Epitaxial Growth of Materials and Structures (OEL)

Growth of the semiconductor layer structures will be performed at OEL with a new low-pressure MOVPE system. OEL will also perform a significant number of tests on the materials before they are delivered to the University of Arizona. These initial tests will be performed with the extensive materials research facilities available at OEL, and will include high-resolution X-ray diffraction, Hall measurements, and photoluminescence spectroscopy.

Prof. Lipsanen's group will design the samples to be used in this task, in close collaboration with Prof. Alan Kost's group. The samples will be of two types. Simple multiple quantum well materials with GaInNAs wells and GaAs barriers will be grown first. Nonlinear absorption and relaxation times will be characterized for these samples using the ultra-fast laser facility described below. Emphasis will be placed on using these samples to gain a fundamental understanding of optical properties of GaInNAs.

The second type of sample will be a semiconductor saturable absorber mirror for mode locking. The saturable absorber medium consists of GaInNAs/GaAs quantum wells and the vertical mirrors are made from AlAs/GaAs layers. The contribution of the team at OEL will include the optimization of growth conditions for the layers in the semiconductor mirrors. Laser light at 1.5 microns can be absorbed by free carriers in the mirrors. Therefore, the effect of doping of the mirror layers will also be studied. Detailed modelling of the potential mirror structures will be used to aid characterization. The emphasis for studies of the structure will be to determine which material properties most affect mode locking.

Task 2: Femtosecond Optical Characterization (OSC)

Professor Axel Schulzgen's group will characterize GaInNAs/GaAs saturable absorbers using an extensive femtosecond laser facility. His laboratory has all the equipment needed to study ultra-fast optics from the ultraviolet to a wavelength of about 3.0 microns. Besides conventional time and spectrally resolved photoluminescence measurements with a spectrometer and streak camera, we will focus on degenerate pump-probe experiments with femtosecond temporal resolution.

Task 3: Mode-locked Waveguide Lasers (OSC and OEL)

Professor Seppo Honkanen's group will design and fabricate the ion-exchanged glass waveguide amplifiers for the mode-locked waveguide lasers. The waveguide amplifiers will be fabricated by a silver film ion-exchange process. Figure 1 shows schematically the waveguide laser configuration. The cavity is formed by attaching a broadband dielectric mirror to the other end of the waveguide and the GaInNAs/GaAs SESAM to the other end. We will design waveguide lasers for 10 GHz and 40 GHz repetition rates. The cavity lengths are about 10 mm and 2.5 mm, respectively. The device operation will be measured by pumping the waveguide at 975 nm wavelength using a high power semiconductor laser diode. Before measuring the actual mode-locked laser output, we will first test the laser properties by using a GaAs/AlGaAs mirror structure without the GaInNAs QW's. The measured output power gives us important information about the intracavity intensity and provides useful feedback for the optimization of the GaInNAs QW structure. The mode-locked output will be measured with a fast detector and the width of the pulses with unique techniques.

2.2 Progress Report

Material study of Ga(In)NAs and growth issues of SESAM structures:

MOVPE growth of dilute nitride materials is complicated and, thus, a wide mapping of basic growth parameters for both GaAsN and GaInNAs was carried out with the low-pressure CCS MOVPE system [45]. Specially, the effects of the growth pressure, different TBAs/III and DMHy/V molar flow ratios and the effect of the choice of the carrier gas (either nitrogen or hydrogen) were studied [11, 12, 22]. GaInNAs QW photoluminescence peaks up to over 1500 nm were measured.

At the same time with the dilute nitride QW optimization process, the growth of AlAs/GaAs Bragg mirrors suitable for SESAMs operating at various wavelengths was optimized. Very high reflectivity was obtained by the mirror structures, see Fig. 2 for a typical structure.

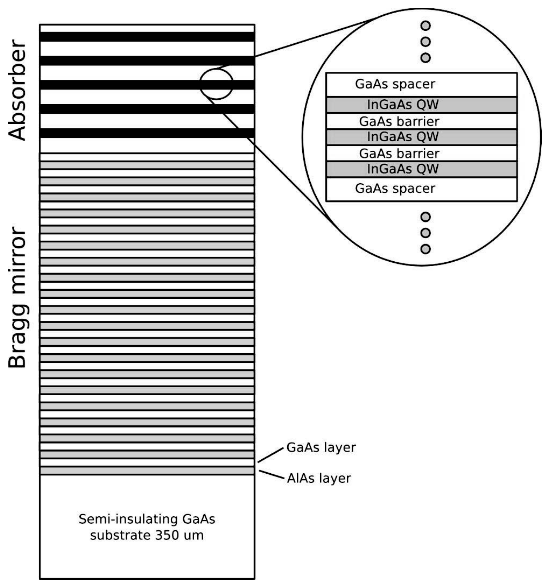

Fig. 2. Example of SESAM structure fabricated by MOVPE.

Anti-resonance operation of the final SESAM structures was desired and it had to be realized by careful structure design. A large number of QWs was required in order to achieve a strong absorption. Therefore, the QWs were placed as 3 or 4 QW stacks at the anti-nodes of the optical field in the cavity. The different stacks were separated by GaAs spacer layers.

As high accuracy of the structure is required for optimal component performance, in situ reflectance monitoring system was utilized. The Bragg mirror growth consisting of thick Al(Ga)As and GaAs layers was monitored as well as the growth of QW structures. By in situ monitoring information about the growth process and the material itself can be obtained. Several papers were published considering the in situ monitoring of the QW MOVPE growth and the high temperature complex refractive indices of Ga(In)NAs [11-12, 18, 20-22].

By now, SESAM structures with operational wavelength at 914 nm, 1064 nm, 1300 nm and 1500 nm have been grown. Mode locking and Q-switching were obtained at 1064 nm by structures having different number of QWs.

Birefringence:

Optical communications networks require integrated photonic components with negligible polarization dependence, which typically means that the waveguides must feature very low birefringence. Recent studies have shown that waveguides with low birefringence can be obtained, e.g., by using silica on Si waveguides or buried ion-exchanged glass waveguides. However, many integrated photonic circuits consist of waveguides with varying widths. Therefore, low birefringence is consequently required for waveguides having different widths. This is a difficult task for most waveguide fabrication technologies. In our work we have demonstrated experimentally low birefringence in buried silver-sodium - ion exchanged glass waveguides [10,15]. Birefringence on the order of 10^{-6} for waveguide mask opening widths ranging from 2 to 10 μm can be obtained by post processing the sample through annealing at an elevated temperature. The measured values are in agreement with the values calculated with our modeling software for ion-exchanged glass waveguides. This unique feature of ion-exchanged waveguides may be of

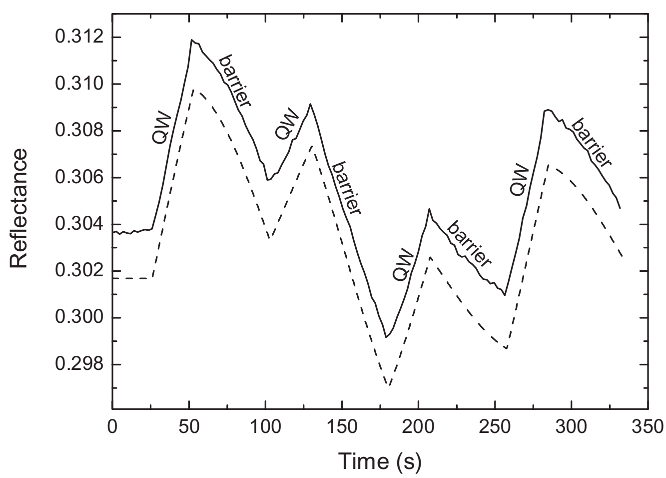

Fig. 3. In situ reflectance curve measured at 635 nm of an InGaAsN/GaAs multi-quantum-well structure during MOVPE growth. [18]

significant importance in a wide variety of integrated photonic circuits requiring polarization independent operation.

Waveguide laser and Q-switching:

We have demonstrated lasing operation in 1-cm long waveguide cavities on phosphate glass doped with varying concentrations of erbium and ytterbium [35]. Waveguides were fabricated by silver film ion exchange process. Unlike molten salt ion exchange processes this is a dry process and its major benefit is that low loss surface waveguides can be easily produced. Waveguides fabricated in this way typically feature a propagation loss below 0.15 dB/cm and a good mode matching with a fiber.

The waveguides were characterized in order to determine the small-signal gain and to demonstrate the laser operation. The measurement setup consisted of a fiber pigtailed diode pump laser at the wavelength of 980 nm with an available output power of 180 mW coupled to the waveguide, a tunable 1550-nm laser, and an optical spectrum analyzer. The measured small-signal gain was approximately 4 dB/cm at signal wavelength (1535 nm). In order to demonstrate the laser operation, the input fiber was coated with a dielectric mirror with reflectivity >98% at the signal wavelength and <5% at the pump wavelength (980 nm). A dielectric mirror with an unoptimized output coupling of 7% was used at the output. The maximum measured output power was 18 mW. The slope efficiency was approximately 11%. The corresponding internal mode intensity is of the order of 10^5 W/cm^2 which is high enough for modelocking a SESAM. The cavity length was chosen so that if integrated with a saturable absorber the combination would produce 10 GHz repetition rate.

Finally, the cavity was combined with a SESAM structure. The pump power was delivered through a fiber coated with a broadband dielectric mirror as described above. This configuration resulted in a Q-switched modelocking in which the modelocked pulses are under much longer Q-switched pulse envelopes. These results were obtained just very recently, and will be published soon. We believe that it is possible to obtain continuous modelocking by reducing the cavity losses and/or optimizing the modulation depth of the SESAM. Large modulation depth is desirable for self-starting modelocking but this easily results in Q-switching instabilities.

Photosensitivity studies and UV-exposed Bragg gratings for laser applications in silver-sodium ion-exchanged phosphate glass waveguides

Waveguide lasers on phosphate glass would benefit greatly if the Bragg gratings providing the optical feedback and wavelength selection could be formed by using UV-irradiation through a phase mask, as is common in fiber optics. Typically, the Bragg gratings required for the optical feedback have been etched in the glass waveguide surface by Ar ion-milling. However, this is a time-consuming and a rather elaborate method. In this work, we presented results on high quality UV-written Bragg gratings in passive Schott IOG-1 phosphate glass channel waveguides. We also reported on a first demonstration of a distributed Bragg reflector (DBR) waveguide laser using a photowritten grating in a hybrid IOG-1 glass [14].

We demonstrated narrowband gratings with high reflectivity in silver ion-exchanged channel waveguides made in Schott IOG-1 glass. High reflectivity Bragg gratings have been written by

ArF excimer laser through a phase mask into Schott IOG-1 hybrid phosphate glass (Fig. 1 a)). After grating exposure, a waveguide was fabricated by silver-sodium ion-exchange. Reflectivities around 80% at a wavelength of ~1535 nm were measured from the waveguide for both quasi-TE and -TM polarizations. Waveguide laser operation with the photowritten waveguide grating as another mirror was demonstrated. Output power of 9 mW with a pump power of 200~mW could be extracted from the laser configuration slope efficiency being 14% (Fig 1b)). The gratings were fabricated in Carleton University (Ontario, Canada) in co-operation with Prof. Jacques Albert. Sanna Yliniemi visited his research group for six weeks in 2005.

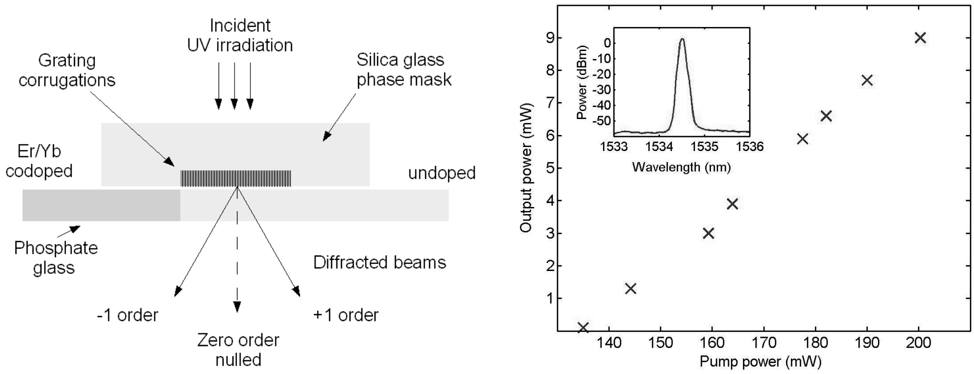

Fig. 4. a) Set-up for the phase mask technique used to fabricate Bragg gratings into glass substrates, and b) slope efficiency and the output spectrum (inset) for a waveguide laser with a UV-written Bragg grating.

A comprehensive study of the origin of photosensitivity in Schott IOG-1 glass was also carried out [13]. Permanent sub-micron-period volume index gratings with modulation amplitude larger than 10^{-4} were obtained even after annealing the irradiated samples for 2 hours at 230 C. Ultraviolet-visible absorption changes were measured in the irradiated areas, as well as structural modifications observed by surface profiling. Comparative studies were carried out for glasses which are co-doped with erbium and ytterbium.

Diluted nitride structures on germanium

Incorporation of nitrogen into GaAs material affects differently on the physical properties of GaAs than in conventional semiconductor alloys. The unusually strong behaviour of the band gap E_g as the composition of N is altered, know as band gap bowing effect may enable telecommunication wavelengths up to 1.55 μm using GaInNAs compounds and is actively studied for use in novel solar cell structures. The GaInNAs structures have been fabricated until now on GaAs wafers. However, germanium substrates are attractive alternatives for this. They are almost defect-free up to large diameter and they have intrinsically lower price than GaAs wafers. Therefore, fabrication of diluted nitrides on Ge was studied in detail [5, 9, 40].

The incorporation efficiency of N into GaInAsN quantum well layers is very low. However, in the new approach were Ge substrates are used instead of GaAs substrates the incorporation efficiency of N was found to be more effective. This enhancement results from the small strain compensation introduced by Ge. Lower wafer surface temperature may also play a role in the higher N composition obtained with Ge substrate [40].

Semiconductor nanowires

Semiconductor nanowires may play an important role in future nanophotonic circuits. Therefore, growth process for catalytic [16] and catalyst-free [17] fabrication of semiconductor nanowires by vapour-liquid-solid (VLS) technique were developed based on gold nanoparticles and in situ deposited indium nanoparticles, respectively. Addition of nitrogen into InP nanowires causes decreased PL intensity but no shift in emission wavelength [19]. A novel method to improve drastically the PL intensity has been recently reported [26].

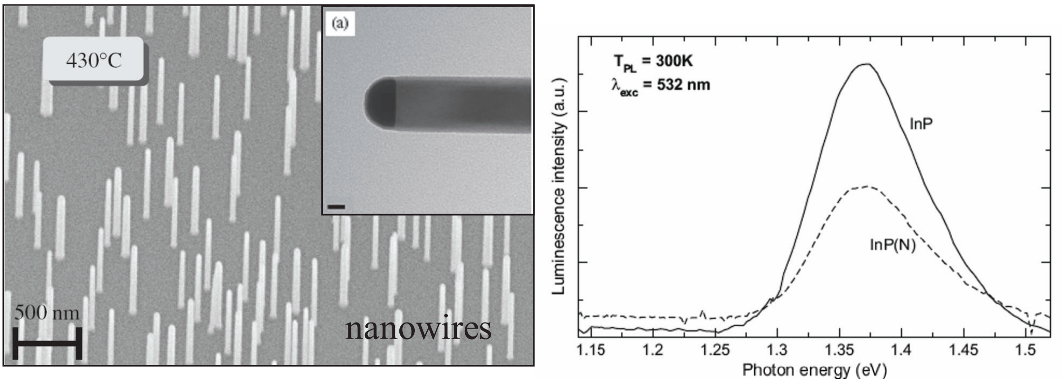

Fig. 5. a) InP nanowires fabricated by VLS growth using MOVPE. b) Room-temperature photoluminescence from VLS grown InP nanowires and diluted nitride InP(N) nanowires. [19}

3 International Aspects

A research visit to the University of Arizona was made by graduate students Outi Reentilä and Marco Mattila during the spring 2005 (from February 21 to March 3) to get in touch with both the measurement equipment designed for the femtosecond optical characterization and the Axel Schulzgen's research group. Harri Lipsanen visited OSC in December 2004.

Ms. Sanna Yliniemi (PhD Student) worked at OSC Arizona from 2003 to 2005. She visited Prof. Jacques Albert's research group in Carleton University, Ottawa, Canada, in May 2005. She carriers on studies with the uv-photosensitivity of passive and active IOG-1 phosphate glass. The final goal is to fabricate DFB laser on active IOG-1 glass using uv-written Bragg gratings. Results on photosensitivity of passive IOG-1 glass were published at 30th Australian Conference on Optical Fibre Technology in July 2005.

A meeting dedicated to diluted nitrides, Workshop on Metastable Compound Semiconductor Systems and Heterostructures, Marburg, Germany, invited Harri Lipsanen to give a talk on “ In situ characterization of dilute nitride quantum wells grown by MOVPE” in December 2006 [37].

Collaboration with professor Naci Balkan, University of Essex, UK, has been fruitful. Two manuscripts on diluted nitrides have been submitted for publication recently [23-24].

4 Publications and Academic Degrees

Table 2. Publications and academic degrees produced in the project. Numbers of different types of publications are given along with the reference numbers. List of refereed journal articles are given in Section 6.1, refereed conference papers in Section 6.2, monographs in Section 6.3 and theses in Section 6.4.

Partner	Type of publication	2003	2004	2005	2006	**Total**	Publication numbers
OEL	Ref. journal art.	-	5	5	15	**25**	1-25
	Ref. conf. papers	2	6	2	6	**16**	26-38
	Monographs	-	-	1	-	**1**	39
	Doctoral dissert.	-	-	-	1(+3)	**4**	40-43
	Licentiate degrees	-	-	-	-	**0**	
	Master degrees	1	-	-	-	**1**	44

5 Other Activities

An article about ultrafast microlaser was published in a Finnish journal, Prosessori (Prosessori, 27-28, November 2004) [45]. The article was written in Finnish and its title was "Valolla vauhtia viestintään (Ultrafast microlaser)". Outi Reentilä, Marco Mattila and Harri Lipsanen from OEL and Sanna Yliniemi and Seppo Honkanen from OSC participated in the writing work. The readers of Prosessori found the work interesting and gained feedback was positive. Laytec GmbH, a German company devoted to in situ monitoring for epitaxy has selected our work as a main topic in their recent news letter [47].

6 Publications

6.1 Refereed Journal Articles

[1] J. Sormunen, J. Toivonen, M. Sopanen, and H. Lipsanen, Morphology of ultra-thin cubic GaN layers on GaAs(100) grown by MOVPE with DMHy as nitrogen source, Applied Surface Science **222**, 286-292 (2004).

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ULTRA-FAST QUANTUM-REGIME SEMICONDUCTORS, COMPONENTS, AND SUB-SYSTEMS (QUEST)

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Abstract

TULE QUEST was concerned with the fundamental research of *quantum-regime optical wavelength-scale semiconductors and devices* to improve the understanding of the physics of *ultra-fast optical phenomena* in solid state matter and to demonstrate the existence of such phenomena in actual devices. The Consortium addressed these issues in many ways: theoretically, experimentally, and technologically. One of the most important achievements was *a breakthrough* made in studies and generation of *ultra-fast (femtosecond) optical pulses produced from fibre lasers* at the technologically important wavelengths (λ) of 900, 1064, and 1550 nm. Other interesting results included an *observation of the single quantum-well walls* almost on an atomic scale, observed for vacuum-cleaved samples by means of a cross-sectional scanning tunnelling microscopy, and the use of the *positron emission spectroscopy and time-resolved photoluminescence* to observe *the effects of ion-irradiation on the dynamics of charge carriers in III-V heterostructures*. A very useful *pump-probe system* for studies of ultra-fast reflectance phenomena was built. Comprehensive theoretical work provided much needed information about the *electronic and optical properties of various types of semiconductors*, notably of GaN and dilute-nitride GaInNAs which are being used as building blocks for blue lasers and LEDs and infra-red telecom devices, respectively. Studies of *photonic crystal (PC) fibres* greatly improved the understanding of the light propagation in these very special lasers.

The Consortium also developed other *novel optoelectronic devices* in full accordance with the original Project Plan. Remarkable results were obtained on a *broadband non-linear mirror*, SESAM, which after ion irradiation exhibited ultra-fast responses to incident light. Using the SESAM, a *high-power ultra-fast mode-locked fibre laser* was developed. Further achievements in studies of photonic devices included a creation of record-wide (1000 nm) *super-continuum radiation* for the visible ("white light") and infrared regimes. Effective *frequency conversion* was also demonstrated for a 1060-nm fibre laser down to 532 and 352 nm. Finally, *synchronous clocking* of two mode-locked fibre lasers (1064 and 1550 nm) was demonstrated.

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Within TULE QUEST, the Consortium produced altogether 23 Master Theses and 15 Doctoral Dissertations, which were at least partly funded by TULE QUEST. The Consortium published altogether 97 scientific papers in international journals, from which 15 were Partners' joint publications.

1 Partners and Funding

1.1 Optoelectronics Research Centre, Tampere University of Technology (ORC/TUT)

The research group consisted of Project Coordinator Prof. Markus Pessa, WP 2 Leader Prof. Oleg Okhotnikov, WP 3 leader PhD Mircea Guina, Senior Researchers Dr. Eero Arola, and Dr. Changsi Peng, Dr. Wei Li, Researchers Dr. Tomi Jouhti, Dr. Suvi Karirinne, Dr. Emil-Mihai Pavelescu, postgraduate students Ilkka Hirvonen, Antti Härkönen, Antti Isomäki, Lasse Orsila, Markus Peltola, Victor Tapio Ragnel Kuoppa, Lauri Toikkanen, Antti Tukiainen, Anne Vainionpää, Jukka Viheriälä, Matei Rusu, Jari Lyytikäinen and students Vesa Erojärvi, Mikko Pekonen, Lauri Rajala, Janne Konttinen, Antti Laakso, Ville Rimpiläinen, Andreas Rydefalk, Risto Rönkkö, Olli Tengvall, Matti Haavisto, Tommi Hakulinen, Kimmo Haring, Esa Saarinen, and Juha Kontio.

1.2 Surface Science Laboratory, Tampere University of Technology (SURF/TUT)

This group consisted of Prof. Mika Valden, Senior Researcher Dr. Mika Hirsimäki, a postgraduate student Kimmo Lahtonen and undergraduates who worked as part-time research assistants.

1.3 Theory Group, Department of Physics, Tampere University of Technology (TCOMP/TUT)

"Theoretical and Computational Materials Physics" Group was led by Prof. Tapio Rantala and assisted by Senior Researchers Dr. Eero Arola and Dr. Jouko Nieminen, postgraduates Ville Arpiainen, Hannu-Pekka Komsa, and Jussi Ojanen, and students Matti Viitala and Ilkka Kylänpää.

1.4 Institute of Materials Chemistry, Tampere University of Technology (IMC/TUT)

This research group was headed by Prof. Helge Lemmetyinen and assisted by Acting Prof. N. V. Tkachenko, Researcher Dr. E.-M. Pavelescu, and a postgraduate V. D. S. Dhaka.

1.5 Laboratory of Physics, Helsinki University of Technology (Phys./HUT)

The research group consisted of a sub-project leader, docent Filip Tuomisto, a senior researcher docent Jonatan Slotte and Dr. Asier Zubiaga, and graduate students Simo Kilpeläinen, Katja Kuitunen, Jussi-Matti Mäki, Antti Pelli, Floris Reurings, Mikko Rummukainen, and Petri Sane. The group also employed two undergraduate students. Furthermore, the former group members who had considerable contribution to TULE QUEST were: Prof. Kimmo Saarinen (deceased), postgraduate students Reino Aavikko, Sami Hautakangas, and Antti Laakso and a few undergraduates.

1.6 COMP / Laboratory of Physics, Helsinki University of Technology (COMP/HUT)

This research group was headed by Prof. Risto Nieminen and assisted by Senior Researchers Dr. Chris Latham and Dr. Maria Ganchenkova, and a postgraduate Katri Laaksonen.

1.7 Accelerator laboratory, Department of Physical Sciences, University of Helsinki (UH)

The research group was headed by Prof. Juhani Keinonen, and assisted by Senior Researcher Dr. Kai Arstila, postgraduate students Kenichiro Mizohata, and student Carolina Björkas.

1.8 Nanoscience Center, University of Jyväskylä (JYU)

The research group was headed by Prof. Päivi Törmä and assisted by postgraduate students Anu Huttunen and Timo Koponen.

1.9 Funding

Table 1. Funding of TULE QUEST in units of 1,000 EUR for the full period of 2003 - 2006. Internal funding includes manpower costs and operational expenditures allocated by the organization itself.

Partner	Funding	2003	2004	2005	2006	**Total**
P1: ORC/TUT	Academy	103.15	167.17	146.86	23.82	**441**
P2: Surf./TUT	Academy	20.48	40.79	38.86	3.43	**104**
P3: TCOMP/TUT	TUT	0	18	18	18	**54**
	Academy	15.15	22.63	21.64	0.58	**60**
P4: IMC/TUT	TUT	-	15	40	15	**70**
	Academy	20	22.5	37.5	0	**80**
P5: HUT	HUT	25	25	25	25	**100**
	Academy	25.8	57.5	52.6	0.1	**136**
P6: COMP/HUT	HUT	20	20	20	20	**80**
	Academy	28	39	33	4	**104**
	Other	10	10	20	20	**60**
P7: UH	UH	32.8	34.2	28	5	**100**
	Academy	22.815	49.082	43.938	4.165	**120**
P8: JYU	Academy	12.056	12.517	8.909	1.517	**35**
Total		**335.251**	**533.389**	**534.307**	**141.053**	**1544**

2 Research Work

2.1 Objectives and Work Plan

Work Plan was made of three Workpackages (WP). They were divided into Tasks, each Task having its specific objectives.

WP 1: High-Speed Semiconductors

Task 1A: X- STM for direct observation of atoms at heterojunctions

Objectives: (i) observe quantum-well intermixing as a function of sample temperature, (ii) atomic vacancies and clustering, and (iii) moving atoms (by snapshots) on the cleavage plane, due to diffusion. Responsible Partner: P2.

Task 1B: Defect production and identification

Objectives: (i) modification of optoelectronic semiconductors by ion beam irradiation, (ii) characterization of the nature of defects produced, and (iii) improving the understanding of physical processes that occur during and after ion implantation and the role of damages in carrier trapping and recovery time of a SESAM. Responsible Partner: P7.

Task 1C: Positron annihilation spectroscopy

Objectives: (i) Year 1: study the formation of point defects in different growth and doping conditions, and investigate the role of N alloying in the point defect formation, (ii) Year 2: study the influence of alloy composition, defect clustering and ion implantation damage in SESAMs, and (iii) Year 3: investigate defects and diffusion, and study correlations with positron spectroscopy, cross-sectional STM and time-resolved PL. Responsible Partner: P5.

Task 1D: Optical femtosecond spectroscopy

Objectives of this Task are to measure ultra-fast transient absorption, reflectance, and PL of heterostructures prepared by P1 and modified by P7. P4 will study the samples with varying (i) composition, (ii) doping concentration, (iii) dose of heavy-ion irradiation, and (iv) annealing conditions. Responsible Partner: P4.

Task 1E: Theoretical studies

Task 1E will be carried out by two Partners: P3 and P6. The modelling and simulation effort is divided into two groups, (i) *first-principles modeling of materials* and (ii) s*imulation of excitations and dynamics.* Both are linked to the other activities of WP1, and are instrumental in optimization of materials properties, in interpreting the experimental results, and in understanding the complex, non-linear behavior of ultra-fast optical response.

WP 2: Ultra-fast components

The overall objectives in this WP were to develop (i) broadband non-linear SESAMs and (ii) high-power mode-locked fibre lasers (MLFL's) operating at the wavelength range of 1.0 and 1.55 μm.

Task 2A: SESAM at 1 μm and 1.55 μm for mode-locking of high power fibre lasers

Objectives: (i) determination of an optimum amount of artificially created recombination centers in a SESAM to reduce its absorption recovery time, (ii) clarification of non-linear absorption and structural properties of ion-irradiated GaAs and InP SESAM's, and (iii) investigation of the role of post-growth thermal annealing in stabilization of operational parameters to eliminate short-lived recombination centers. Responsible Partner: P1.

Task 2B: SESAM-based high-power mode-locked fibre lasers

Objectives: develop a reliable mode-locked fibre laser capable of generating ultra-short optical pulses at high power. A major goal is to demonstrate a light source, which emits pulses with sufficient energy to be able to saturate the gain of a high-power amplifier. Responsible Partner: P1.

WP 3: Ultra-fast sub-systems

Tasks 3A-3C: Demonstration of ultra-fast, high-power optical sub-system. Target: output power up to micro- or millijoule for sub-ps pulses.

Objectives: (i) design and demonstrate efficient amplification of ultra-short optical pulses, (ii) to investigate theoretically micro-structured fibres as non-linear, dispersive and amplifying media, and (iii) to generate super-continuum (SC) radiation in optical fibres and wavelength conversion through second-harmonic-generation. Responsible Partner: P1.

2.2 Progress Report: Common Themes and Collaboration

We wish to emphasise that there was a fruitful and close cooperation between the Partners in TULE QUEST. This is evidenced by 15 joint publications in high-impact international journals. [1], [7], [10-12], [14-15], [20-21], [23], [25-27], [29], [86]

General: Material growth and characterization

Multi-technique characterisation of the materials, which were grown by ORC, or occasionally acquired outside the Consortium, included ion-irradiated quantum-well laser and SESAM structures. Ion-irradiation was performed by Accelerator Laboratory of UH. Irradiated samples were studied by the Institute of Materials Chemistry (IMC) of TUT, the Laboratory of Physics of HUT, and ORC.

IMC accomplished construction of a pump-probe ultra-fast measurement system, which could be used to measure femtosecond reflectance transients in semiconductor heterostructures. Besides the time-resolved PL and pump-probe measurements, a number of samples were sent to the Laboratory of Physics of HUT for studies of positron annihilation spectroscopy (PAS). This Laboratory, HUT, also investigated other samples acquired from abroad (e.g. GaN samples) using PAS.

Many of the results of this workpart were published in the international literature [1–3], [9–11], [13–16], [22–27].

Recovery dynamics and non-linear response in ion-irradiated and annealed semiconductor saturable absorber mirrors

Optical properties of the saturable absorber mirrors, which were either as-grown, heavy-ion or light-ion irradiated and then annealed, were examined. An important outcome was the finding of closely optimal conditions for ion-irradiation and thermal annealing. This finding helped control the absorption recovery time and improved non-linear properties of the mirrors. It could be shown that irradiation with 10^{12} cm^{-2} of 6-MeV Ni^{+}-ions and 1-sec annealing at 400 °C led to the absorption recovery time of a few picoseconds. The modulation depth corresponded to 95 % of the one of the non-irradiated sample. Non-saturable losses decreased by 45 %, when compared to losses occurring in the irradiated, non-annealed absorbers.

The SESAMs were grown by MBE on *n*-type GaAs (100) substrates. They were irradiated at UH with 6-MeV Ni^{+}, Ne^{+}, He^{+}, H^{+}-ions at doses of 10^{10} to 5×10^{12} cm^{-2} for the heavy ions (Ni^{+} and Ne^{+}) and up to $\sim 10^{14}$ cm^{-2} for the light ions. We were able to determine approximately optimal annealing conditions for the SESAMs, while keeping the recovery times at a level acceptable for mode-locking fibre lasers. The latter requirement was of crucial importance for achieving and maintaining passive mode-locking.

Fig. 1 shows evolution of reflectivity of a SESAM as a function of incident pulse energy for as-grown, ion-irradiated (6-MeV, 10^{12} cm^{-2}), and annealed samples (100 °C for 1-sec and 400 °C for 1 sec). For annealing at 400 °C, the non-linear reflectivity bore close resemblance to that of the as-grown sample. Based on the data obtained (see Table 2), one can conclude that annealing at 400 °C recovered the modulation depth of an irradiated sample almost completely (i.e., 95 % of the modulation depth) and, importantly, decreased non-saturable loss by 45 % compared to an irradiated non-annealed sample.

Table 2: Summary of the properties of SESAMs upon post-growth treatments

Sample	**Non-saturable loss**	**Modulation depth**	**Saturation fluence**	**Recovery time**
As-grown (no further treatment)	8.7 %	18.3 %	3.3 μJ/cm²	162 ps
Irradiated, no annealing	19.5 %	14 %	4.5 μJ/cm²	0.8 ps
Irradiated, annealed at 100 °C, 1 sec	15 %	15 %	4.8 μJ/cm²	0.8 ps
Irradiated, annealed at 400 °C, 1 sec	11 %	17.4 %	2.9 μJ/cm²	1.1 ps

In summary, (i) optical properties of ion-irradiated SESAMs could be recovered almost completely by annealing upon ion-irradiation; (ii) annealing retained a desired reduction in recovery time caused by ion irradiation. *We now have a practical method at hand* to treat a SESAM after growth in order to obtain a desired modulation depth and very small non-saturable loss (this loss is undesired). *This achievement has had an immediate consequence applicationally, because it enables us to build mode-locked ultra-short-pulse fibre lasers.*

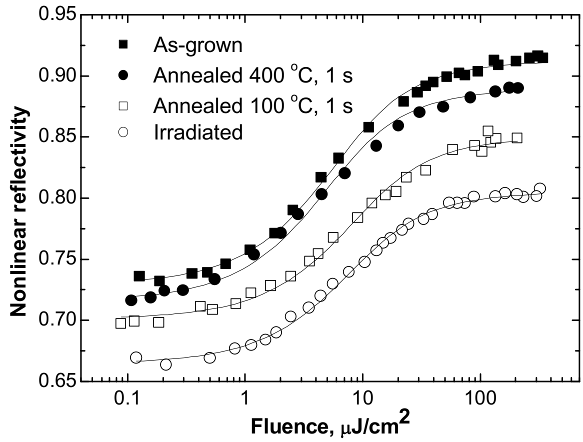

Figure 0. Non-linear reflectivity of SESAMs before sample irradiation, after 10^{12} cm^{-2} Ni ion irradiation at the energy of 6 MeV, and after annealing for 1 sec at 100 °C and 400 °C.

X-STM-related issues

In this Task, cross-sectional STM (X-STM) was carried out for GaInNAs (100), cleaved along the (110) crystallographic plane, resulting in almost atomically flat surfaces. The cleavage could be made *in situ* under ultra-high vacuum. Therefore, the exposed surface remained free of surface contamination long enough for the measurements. Yet, the cleavage process itself was challenging because it induced some structural defects and never resulted in a large, atomically flawless surface.

The cleavage was initiated by making a notch on a sample edge. Since there was no appropriate scriber at Surface Science Laboratory to prepare the samples for cleaving, the Laboratory used three different scriber systems: two at ORC (both were inaccurate yielding poor cleavage) and one at Coherent Finland Ltd. It turned out that all the scribers were inadequate to control the length and depth of the scratch in such a reproducible and accurate fashion that is needed for the cross-sectional STM experiments.

Despite unexpected difficulties, we were able to make some quite successful X-STM profiles of the cleaved surfaces of GaInNAs QWs (Fig. 2, Sample #AsN 659).

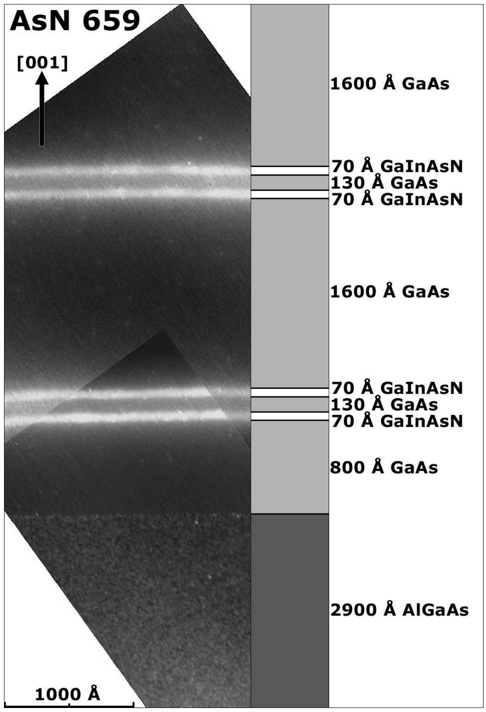

Figure 2. High-resolution X-STM image of the GaInNAs four quantum wells grown on an *n*-GaAs(001) substrate, obtained with 338 pA tunnelling current and -2.07 V sample bias voltage. The colour-scale range displayed is 0.73 nm.

Since STM physically represented contours of a constant integrated charge density, the quantum wells could readily be resolved by sharp protrusions in the X-STM image (the yellow stripes in Fig. 2). Because further interpretation of the results was needed we asked TCOMP/TUT to make STM simulations for the samples.

Time resolved studies of GaInNAs / GaAs and GaInAs / InP QW structures

Substantial part of TULE QUEST was concerned with time resolved luminescence and pump-probe studies on as grown and ion-irradiated compound semiconductor samples. We wanted to understand the physical phenomena that govern the dynamical processes in heterostructures, particularly in quantum wells, which are the active media in LED's, lasers and other photonic components.

The PL up-conversion Technique

A schematic diagram of the basic principle of the parametric up-conversion technique is shown in Fig. 3. After an ultra-short pulse excites the sample, the luminescence from the sample is collected, collimated, and combined with part of the excitation pulse in a non-linear crystal such as BBO_3. The angle of the crystal is set in order to phase-match the sum frequency generation for the gating pulse and sample luminescence. The signal at sum frequency is recorded by a detection system consisting of a colour rejecting filter, monochromator and photomultiplier operating in photon counting mode. By varying the delay of the gating pulse and measuring the sum frequency signal, the temporal profile of the luminescence is obtained with no background signal. Since up-conversion involves virtual electronic transitions, this gate has a response time in femtosecond time scale.

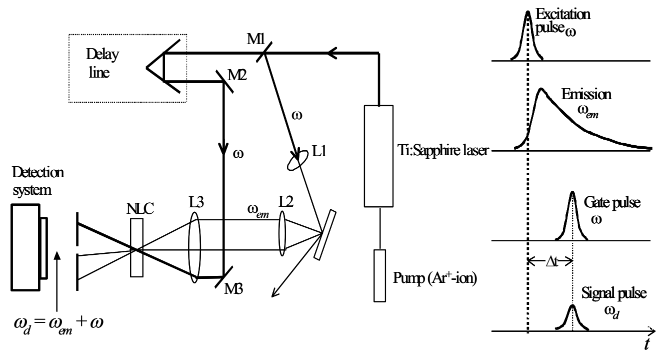

Figure 3. Scheme for PL up-conversion technique

A femtosecond self-mode-locked titanium sapphire laser, pumped with an argon ion laser, was employed as a source of excitation pulses. The pulses had the wavelength of 820 nm, the pulse width of 50 fs, the repetition rate of 90 MHz. The time resolution of the system is ~100 fs. The excitation power is 20 - 30 mW, i.e. the optical energy density on the sample surface was ~0.3 mJ/cm^2.

Three types of MBE-grown QW structures were studied by TRPL: (a) **InGaAs/GaAs** consisted of five compressively strained QWs made of 6 nm thick $In_{0.29}Ga_{0.71}As$/17 nm GaAs heterostructures, which were deposited onto a 200 nm GaAs buffer layer on a GaAs(100) substrate and capped with a 100 nm GaAs layer. (b) **InGaAs/InP** consisted of an InP buffer layer of 100 nm in thickness, deposited onto an *n*-type InP(100) followed by growth of seven $In_{0.576}Ga_{0.424}As$/InP QWs, each 6 nm in thickness and separated by 8-nm InP barriers. The whole structure was capped with a 100-nm InP layer; all layers were nominally undoped. (c) **InGa(N)As/GaAs:** here two $Ga_{0.63}In_{0.37}As$/GaAs QW and two $Ga_{0.63}In_{0.37}N_{0.011}As_{0.989}$ / GaAs samples were grown on *n*-type GaAs(100) substrates. The heterostructure contained a 100-nm GaAs buffer layer, a 30-nm GaAs barrier layer, 10 GaInAs (or GaInNAs) QWs each with 6 nm in thickness, and a 100-nm GaAs cap layer on the top.

Barrier and QW carrier dynamics

Photo-excitation of the layer structure, such as InGaAs / GaAs, was carried out with the excitation wavelength shorter than the barrier band gap (see Fig. 4) to create free carriers all over the sample.

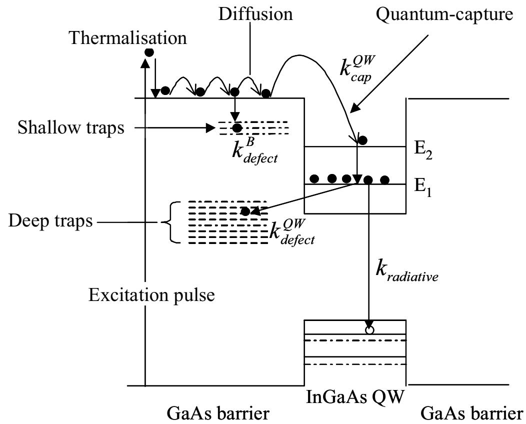

Figure 4. Schematic representation for capture and decay dynamics of electrons in (ion-irradiated) InGaAs / GaAs QW structure upon photo-excitation.

After very quick thermalization of photo-excited carriers in the barrier, the motion of carriers proceeds stepwise: (1) drift and diffusion in the barrier layer, (2) quantum capture by the QW, (3) fast relaxation within the QW states (*i.e.* E_2-E_1), and finally (4) decay in the QW due to non-radiative (*via* defect states) or radiative recombinations. At room temperature, the radiative recombination is almost negligible.

Only those carriers that reach the QW contribute to the QW carrier dynamics. The carriers created in the cap or barrier far away from the QWs do not reach the QWs before they are trapped by defects or are recombined, so they have no influence on the QW carrier dynamics. Since the thickness of the barrier layers are much larger than that of the QWs, a majority of the photo-excited carriers are generated in the barriers.

Ion implantation creates defects in semiconductor heterostructures. Shallow traps denote those defects located near the barrier / QW interfaces. The defects are created deep enough, *i.e.,* far below the barrier conduction edge, and are denoted as deep traps (shown in Fig. 3). In our samples, heavy ions at high implantation energies were likely to form a majority of deep traps. As the irradiation doses were increased, the shallow traps affected the capture dynamics; therefore, the decay dynamics was governed by the deep traps located inside or near the QWs.

If the barriers were sufficiently thin, so that the carriers could be created near the QWs, carrier diffusion in the barrier could be neglected. It is known that diffusion would play a dominant role only if the barrier thickness between the QWs exceeded 50 nm. In the present work the barriers were thinner than 20 nm, i.e., any contribution from diffusion was marginal.

The hole capture is faster than the electron capture. Thus, the electron dynamics is the time limiting process for luminescence decay. In Ref. [31], equations describing the dynamics of carrier populations in QW structures have been derived. The main result was that in the QW structures the TRPL rise and decay profiles, i.e., the time dependence of the luminescence intensity $I(t)_{PL}$, can be described by a two-exponential curve written as

$$I(t)_{PL} = a\left(e^{-k_{cap}^{eff}t} - e^{-k_{defect}^{QW}t}\right), \qquad (1)$$

where $a=\frac{N\,(k_{cap}^{eff})}{k_{defect}^{QW}-k_{cap}^{eff}}$ and $k_{cap}^{eff}=(k_{cap}^{QW}+k_{defect}^{B})$. k_{cap}^{QW} is the capture or trapping rate of the carriers in the barriers by the QW and k_{defect}^{B} is the non-radiative recombination rate of carriers in the barrier layer *via* defects (native or implantation induced). The negative term in above equation represent the PL rise time τ_{rise} and the positive term corresponds to the PL decay time τ_{decay} or lifetime. Which term is negative depends, whether $k_{defect}^{QW} < k_{cap}^{eff}$ or $k_{defect}^{QW} > k_{cap}^{eff}$.

Effect of excitation energy density on peak PL intensity and lifetime

We (P4) examined the excitation energy density *versus* PL peak intensities and carrier lifetimes for as-grown samples and irradiated InGaAs / GaAs and InGaAs / InP, all grown by P1. The relation between PL peak intensity and excitation power is

$$I_{PL} = \eta E_{ex}^{\gamma}, \qquad (11)$$

where I_{PL} denotes the peak PL intensity, η represents the PL efficiency including the capture, ionization, and recombination processes of the carriers, E_{ex} is the excitation power, and γ describes the parameter determined by radiative recombination.

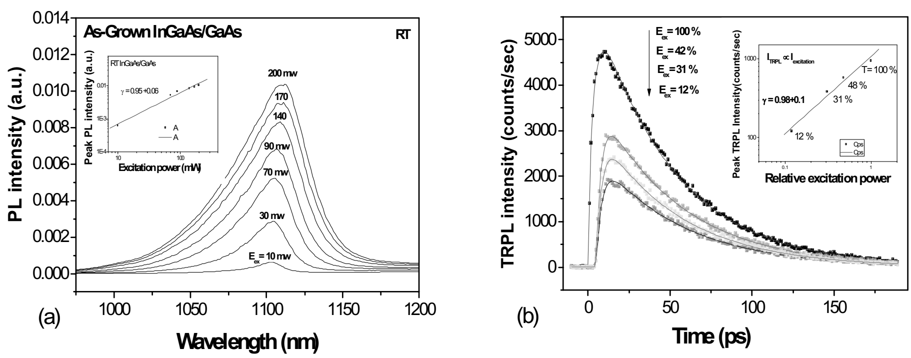

Figure 5. (a) Dependence of PL peak intensity on the excitation power. (b) Dependence of peak TRPL intensity on the relative excitation power.

In our experiments, steady state PL peak intensity (Fig. 5a) and peak TRPL intensity (Fig. 5b) show a nearly linear dependence on excitation intensity, indicating that *the dominant mechanism of radiative recombination at room temperature is excitonic*. It should be noted, that the non-radiative recombination prevails at room temperature.

The carrier decay time τ_{decay} was found to be independent on excitation intensity (see Fig. 5b). As the excitation intensity decreased the lifetimes remained essentially the same. This observation indicated that *the radiative decay was due to monomolecular recombination* and that the QWs were not saturated by the excitation.

Capture and decay of carriers in Ni^+-irradiated InGaAs/GaAs quantum wells

To investigate heavy-ion irradiation *versus* carrier dynamics, InGaAs / GaAs QWs samples were irradiated by 10 MeV Ni^+ with doses (ϕ) at (1-50) × 10^{10} ions cm^{-2} [31].

The formation profiles of PL from the QWs are shown in Fig. 6a. Intensity decreased systematically, as the ion dose was increased, and the decay profiles remained exponential at all doses. The exponential nature of the intensity contour suggested that the time-limiting step in filling the QW was not diffusion from the barriers, *but direct quantum capture by the QW.*

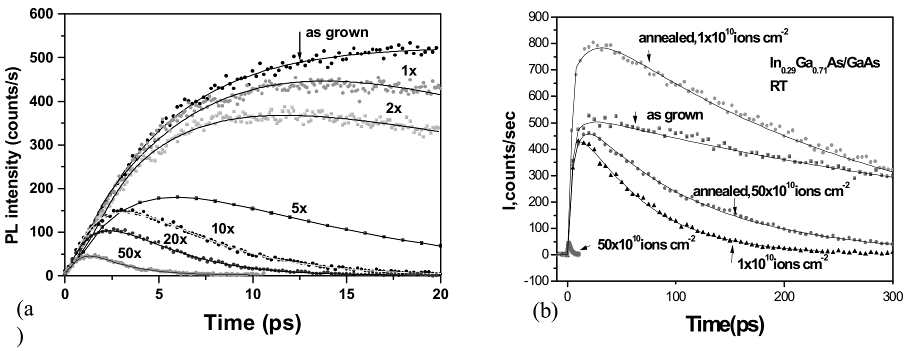

Figure 6. (a) TRPL rise profiles of carriers in InGaAs/GaAs exposed to different Ni^+ doses (indicated in 10^{10} ions cm^{-2}) and (b) effect of irradiation and post-annealing on TRPL decay profiles of few selected samples.

All the samples showed almost similar effective capture times, 4.5 ps, after RTA independent of the irradiation dose. For the highest irradiated sample the capture time was from 2 - 4.4 ps after RTA.

Ni^+-irradiation was very effective in achieving sub-picosecond lifetimes in InGaAs / GaAs. The lifetime reduced from 460 ps for an as-grown sample to 0.62 ps for the highest irradiated sample. The short lifetimes were the results of creation of many ion-induced deep defects, which acted as non-radiative recombination and trapping sites for carriers in the QW.

Studies made in TULE QUEST showed that the lifetimes of the as-grown QW samples were not much affected by RTA. For irradiated samples, RTA removed defects substantially: τ_{decay} for the lowest irradiated sample increased from 62 ps to about 270 ps, while for the highest irradiated sample RTA improved the lifetime remarkably from 0.6 ps to 109 ps.

RTA removed mainly deep traps, which was confirmed by an increase in τ_{decay} after annealing. Annealing had only a mild effect on the capture time.

Thermal instability of defects: room temperature ageing

One of the highlights was the observation that *Ni^+-irradiated defects were thermally unstable during a prolonged time period after irradiation* [32].

Surprisingly, the τ_{decay} of the fresh sample increased by two-fold when TRPL measurements were repeated 45 days after the initial lifetime measurements. Repetition of the experiments after 60 and 100 days showed no further increment in lifetimes. Obviously, about one half of the defects were removed by 45 days of ageing; thereafter the samples remained stable. We call this phenomenon room-temperature self-annealing of defects (or an ageing process). On the other hand, defects were stable for the annealed samples; no changes in their lifetime were found after irradiation.

These results were important for device designers, as any change in recovery time would make device dynamics unpredictable.

Effect of ion implantation energy

Fig. 7a displays the dependence of τ_{decay} on the implantation energy for InGaAs / GaAs QWs at a fixed dose of 5×10^{10} ions cm^{-2}, which shows that τ_{decay} depended upon implantation energy.

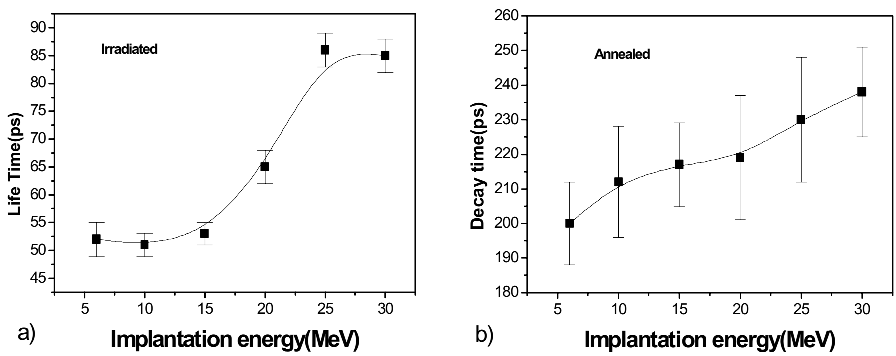

Figure 7. Variation of τ_{decay} with the implantation energy in InGaAs/GaAs QW sample at a fixed Ni^+ dose of 5×10^{10} ions cm^{-2} (a) before annealing and (b) after annealing.

τ_{decay} increased from 52 to 85 ps, as the implantation energy increased from 6 to 30 MeV. This occurred because for the increased energy the amount of nuclear deposited energy in the active region decreased. At high energies, ions got implanted deep inside the GaAs substrate, causing less damage in the epi-layers than would low-energy ions do. This explained the increase in τ_{decay} with implantation energies.

The values of τ_{decay} upon annealing are shown in Fig. 7b. They depended on annealing, and they increased from 52 to 200 ps for the sample implanted at 6 MeV, while the increment was 85 - 238 ps when irradiated at 30 MeV. However, $\tau_{capture}$ depended neither on implantation energy nor annealing after ion implantation. It was 2.5 ps for all the samples.

Effect of light and heavy ion-irradiation

Effects of Ni^+, Ne^+, He^+, and H^+ irradiation on carrier capture and decay in InGaAs / GaAs QWs were measured [33]. The implantation energies were chosen so that they had about the same stopping range profile, and all the ions pass through the active region.

Effective $\tau_{capture}$ for He^+ and H^+ was almost independent of the irradiation dose, while for Ne^+ and Ni^+ it decreased with the dose. The fastest carrier population in the QW was for Ne^+ irradiation; with $\tau_{capture}$ of only 1 ps. $\tau_{capture}$ for the light ions was about 3.5 ps.

Irradiation with the light ions was as effective as that with the heavy ions regarding τ_{decay}, but for the similar nuclear energy deposition and penetration depth profiles much higher doses were required for the light ions to yield the same carrier lifetime [33].

Studies on the τ_{decay} as a function of nuclear deposited energy were also studied. For the same nuclear deposited energy, each irradiation resulted in different τ_{decay}. This suggested that τ_{decay} depended not only on the deposited energy but also on specific kinds of defects produced. It is known that light ions create isolated point defects; the heavier ions produce clusters of defects. While comparing Ni^+ and Ne^+-irradiation with one another, the carrier lifetime and doses appeared to be about the same.

Capture and decay of carriers in InGaAs/InP quantum wells

Effect of Ni^+-irradiation and RTA

The effect of Ni^+-irradiation and post-annealing on $\tau_{capture}$ and τ_{decay} was investigated for InGaAs / InP QWs [34]. $\tau_{capture}$ decreased with the dose, being 8 ps for an as-grown sample and 2 ps for the sample irradiated at the 50×10^{10} ions cm^{-2} level. Annealing had no influence on $\tau_{capture}$.

Since annealing affected τ_{decay} significantly – but not $\tau_{capture}$ – it could be argued that defects responsible for the barrier carrier relaxation were different from those affecting the QW carriers. This meant that the shallow defects were produced near the barrier and QW interface, affecting $\tau_{capture}$, while the deep traps did not much alter capture dynamics, but they were crucial for the QW carrier relaxation (as schematically presented in Fig. 4).

τ_{decay} decreased rapidly, as the dose increased. For the as-grown QW, τ_{decay} was very long, 1.19 ns, but was only 3.7 ps for the highest irradiated sample. Annealing caused no change in dynamics of the as-grown sample, but recovered defects of the irradiated sample.

Fig. 8a displays steady-state PL intensities plotted against irradiation dose. Steady-state PL intensity decreased rapidly, as the dose increased. This correlates well with the TRPL decay curves which exhibit a rapid decrease in lifetimes and TRPL intensities. Annealing recovered defects partially. Fig. 8b shows XRD patterns of an as-grown sample and a sample irradiated at ϕ = 1 × 10^{10}, 10 × 10^{10}, and 50 × 10^{10} ions cm^{-2}. The difference in SL satellite peaks on both sides of the main peak suggests that small structural changes took place at higher doses. Some changes in Ga mole fraction would also be possible, due to possible intermixing at higher doses. These small changes in alloy composition might accelerate the carriers' trapping by the QW and could influence the capture dynamics.

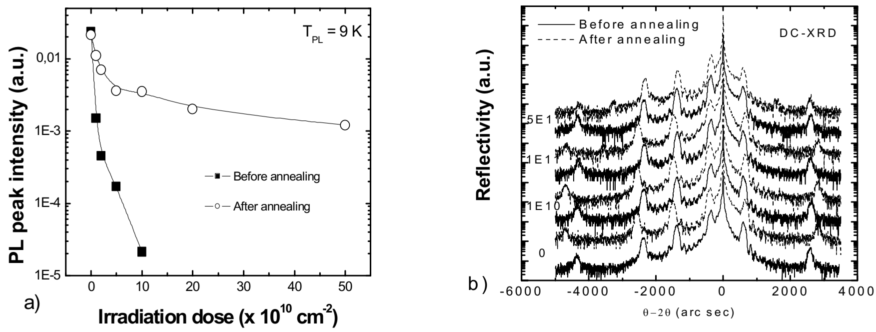

Figure 8. (a) Low temperature PL peak intensities as a function of the irradiation dose and (b) XRD rocking curves for the as-grown and the samples irradiated at different doses, before and after

Effect of ion implantation energy

The PL lifetime increased systematically from 15 ps to 37 ps in the energy range from 6 to 25 MeV. This behaviour could be understood in terms of nuclear deposited energy (in units of eV/ion/Å), since the damage produced in InP and GaAs is dominated by nuclear collision processes for ions in this range (track formation becomes significant only at higher electronic deposition).

The nuclear deposited energy in the active region was determined using the SRIM2003 computer code by calculating the energy transferred to recoil by an incoming ion in the active region in the depth range from 100 to 200 nm. The result was averaged over the InP and InGaAs multi-layer parts (below the top 100 nm InP layer) and is given in Fig. 13. The results reveal that the nuclear deposited energy decreased with increasing implantation energy, and this trend was almost exactly opposite to the change in lifetime. Less damage is correlated with longer lifetimes. Accordingly, *to produce defects, low implantation energies* (less than 5 MeV for Ni^+) are preferred [34].

TRPL Dynamics of GaIn(N)As / GaAs QWs

Effects of growth temperature and rapid thermal annealing (RTA) on the PL rise and decay dynamics of carriers in $Ga_{0.63}In_{0.37}As$ / GaAs and $Ga_{0.63}In_{0.37}N_{0.011}As_{0.989}$ / GaAs quantum well samples were investigated. The GaInAs/GaAs QWs, grown at temperatures (T_{gr}) of 420 °C and 460 °C, exhibited similar PL rise times (τ_{rise}) on an order of 3.5 ps. RTA at 610

^{o}C for 60 s had not much influence on τ_{rise}. On the other hand, τ_{decay} depended on T_{gr}, increasing from 439 ps to 517 ps for the sample grown at T_{gr} = 420 ^{o}C and T_{gr} = 460 ^{o}C, respectively.

Alloying 1.1 at-% N with GaInAs strongly influenced the carrier dynamics. τ_{rise} and τ_{decay} for GaInNAs / GaAs were about 1.0 ps and 11 ps, respectively, when the sample was grown at 420 ^{o}C, and 1.0 ps and 15 ps for T_{gr} = 460 ^{o}C. Incorporation of N created additional defect centres. Shorter τ_{rise} observed in N containing samples was due to the trapping of carries by defect states near the barrier layer rather than the fast capture of electrons by the QW. This is confirmed by about a 107-folded quenching in the steady state PL intensity and only about 40-folded decrease in τ_{decay} upon incorporation of N for the T_{gr} = 420 ^{o}C sample.

RTA reduced structural defects particularly for the lower growth at T_{gr} = 420 ^{o}C, suggesting the carrier lifetime of 70 ps upon RTA treatment. For the T_{gr} = 460 ^{o}C sample the lifetime was 40 ps after RTA. The longer lifetime for the low-T_{gr} sample suggested that low T_{gr} should be favoured if the sample were to be subjected to post-growth RTA.

In summary, the incorporation of N in GaInAs could be an alternative to ion irradiation as to achieving short lifetimes. For GaInAs, the lower the T_{gr}, the smaller the τ_{decay}. For GaInNAs, T_{gr} should be low enough for RTA to recover more defects.

Positron annihilation measurements

One of the common themes of the Consortium was to identify point defects in InGaNAs, and modifications of defects by ion implantation, especially for the SESAMs. The work of the positron group, HUT, was the following. Special sample structures for the positron annihilation spectroscopy were designed, and these samples were grown at ORC. The samples resembled SESAM structures, but different combinations of GaInNAs were fabricated in order to study effects of N and alloying on defect formation. T_{gr} and sample annealing were studied, according to the original work plan.

All samples were measured by the Doppler broadening spectroscopy with the low-energy positron beam. The results indicated that while samples without N exhibited very little defects, the presence of N generated vacancy-type defects. The defect concentration increased when annealing superlattice structures, but in single GaAsN or GaInNAs layers the vacancy concentrations decreased upon such treatment [43]. This interesting difference was attributed to lattice strain in the superlattices and associated defect generation in annealing. *Three journal articles were published jointly with Partners on these observations.*

A set of samples were designed and fabricated for radiation damage studies on the SESAM structures. These samples were measured with a low-energy positron beam. Our preliminary results clearly indicated defect generation by implantation, and might be identified as vacancy-related centres. A manuscript is being prepared on these studies at the time of writing this Report.

Irradiation and ion-beam techniques

The UH group performed high-energy heavy-ion irradiations for the samples prepared by the other Partners (as already discussed to some extent; here, further information will be given). Suitable incident ions, energies, and irradiation doses were chosen using the computer simulations. More than 100 samples were irradiated during the TULE QUEST. High-energy heavy-ion irradiation effects on QW structures are illustrated in Fig. 14. Main results obtained in irradiations were already discussed in the TRPL Section. The τ_{decay} for the QWs decreased as a function of irradiation fluence and deposited energy for different incident ions.

The deposited energy was obtained in computer simulations (SRIM2003) of ion irradiations. A desired τ_{decay} decrease was obtained with all the ions used. For the heavy ions used a much smaller number of incident ions were needed to create the same deposited energy and τ_{decay} effect than what was obtained with the light ions. Computer simulations revealed that the defects responsible for τ_{decay} of the QW depended on ion species: *the heavier ions created more cluster defects, while lighter ions created predominantly isolated point defects*.

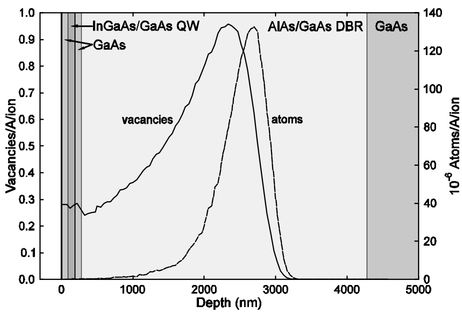

Figure 9. An example of simulated vacancy and range distributions of high-energy heavy-ion irradiation of a SESAM. The incident ion in this simulation is 6-MeV Ni^+. At the depth of the QW absorber region the vacancy density is 0.25 vacancies / Å / ion, while the average penetration depth is about 2.5 μm.

2.3 Progress Report: Progress by Optoelectronics Research Centre, TUT

Optical properties of GaInNAs / GaAs quantum wells

Thermal annealing affected PL emission and x-ray diffraction from GaInNAs / GaAs QW samples. The uncoated samples exhibited a saturable blue-shift of 22 meV relative to PL from the as-grown samples. This shift was attributable to a change in the nearest neighbours of nitrogen in short-range-order N-In_mGa_{4-m} ($0<m<4$) clusters at a fixed composition with negligible Ga / In / N interdiffusion across the junctions. *An insertion of a Si_3N_4 cap layer effectively prevented the blue-shift* in the early stage of annealing and improved emission intensity in contrast to a SiO_2 cap, which is often used in the literature to prevent group-V out-diffusion from semiconductor surfaces during annealing. With SiO_2, out-diffusion was prevented, indeed, but the blue shift was not!

Under high-temperature long annealing conditions (~750 °C, 1500 s), the maximum blue-shift for the Si_3N_4-covered samples was 31 meV. An insertion of a SiO_2 cap layer, instead, caused a large non-saturable blue-shift due to annealing, almost 100 meV. *This large shift was assigned to the formation of Ga -vacancies at the SiO_2 / GaAs interface*. The defects were believed to diffuse into the bulk at elevated temperatures and assist Ga / In / N interdiffusion, which is actually a well-known defect-assisted diffusion process according to the literature.

Semiconductor saturable absorber mirrors (SESAM's) and fibre lasers

ORC demonstrated SESAMs operating at λ = 980, 1060, and 1550 nm suitable for use in Yb- and Er -doped fibre lasers. A Nd-doped mode-locked fibre laser at $\lambda \approx$ 900 nm was developed, too [5], to produce optical pulses with hundreds of femtoseconds long.

Our rapid advance in the SESAM technology within TULE QUEST helped develop passively mode-locked fibre lasers. Recently, we reported pulse sources covering a large wavelength range from 895 to 1560 nm. Mode-locking and stabilization required implementation of the active or hybrid mode-locking techniques. Two-colour sources also appeared to be valuable instruments for ultra-short-pulse optical research, including difference-, harmonic-, and sum-frequency generation, coherent anti-Stokes Raman scattering microscopy, and two-colour pump-probe investigations. A relative jitter between the pulses is a crucial factor, which may severely limit the performance of the laser system. Various schemes for synchronization of ultrafast solid-state lasers with different wavelengths have been attempted by other researchers in the world, but all these solutions have suffered from drawbacks that limit their applications.

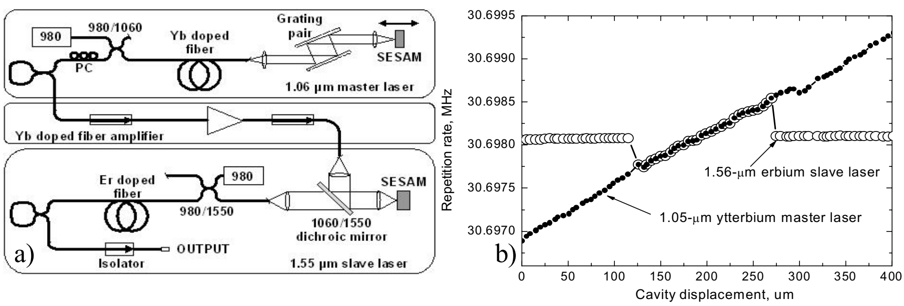

Figure 10. Configuration of the SEMM-synchronization setup (a); round trip frequencies of Er and Yb fibre lasers (b).

Our Consortium demonstrated a novel technique for mode-locked fibre laser stabilization. This technique was based on non-linearity of the semiconductor modulator mirror (SEMM) [6], [9]. Short interaction length and high non-linearity of the semiconductor material allowed for enhanced modulation depth and, consequently, for tight laser synchronization. The stabilization technique of ORC is believed to be suitable for various mode-locked fibre lasers for applications that require low-jitter, ultra-short-pulse oscillators. The saturable absorption phenomenon was exploited in the modulator SEMM. The setup is shown in Fig. 10a. *The ytterbium master-laser (λ = 1060 nm) and erbium slave-laser (λ = 1550 nm) interacted only in the SEMM, providing a very robust pulse locking mechanism.*

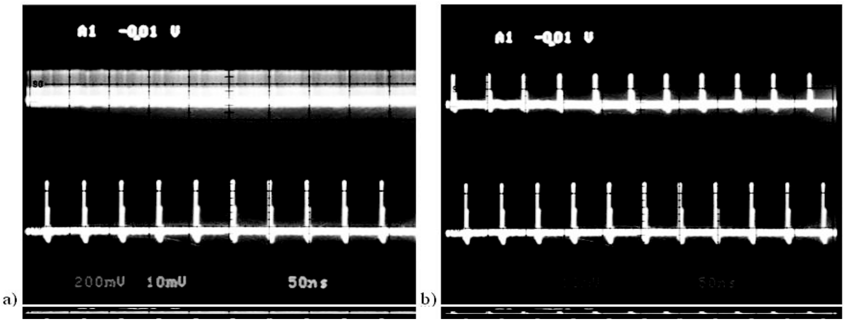

Figure 11. Oscilloscope traces of the pulse trains from erbium (top) and the ytterbium fibre (bottom) lasers in (a) unlocked and (b) synchronized state. The oscilloscope is triggered by the Yb master oscillator.

Detuning the slave laser cavity made it possible to monitor the pulse repetition rate and confirm pulse mode-locking (i.e., coincidence of the frequencies of the slave laser and master laser), as shown in Fig. 10b.

Fig. 11 shows oscilloscope graphs of locked and unlocked pulse trains. The pulse trains provide clear-cut evidence for achieving robust synchronization between the two mode-locked fibre lasers.

Second-harmonic generation

Second-harmonic generation (Fig. 12) from a 1060 nm mode-locked fibre laser was demonstrated within TULE QUEST. A record-high average power of 50 mW at 532 nm (green) was obtained with a conversion efficiency of 30 %. We also succeeded in third-harmonic generation of the same laser and produced UV-blue light at $\lambda = 352$ nm (Fig. 13 and Ref. [120]).

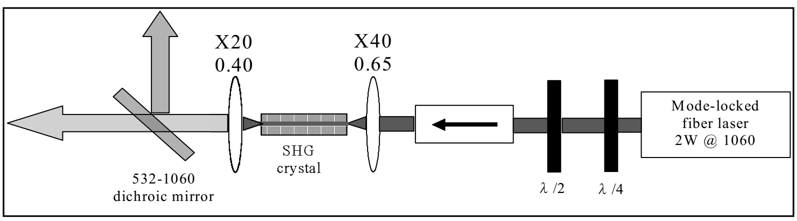

Figure 12. A schematic view of second-harmonic generation process. The pump laser parameters: Average power = 2 W, Wavelength = 1060 nm, Pulse energy = 20 nJ, Pulse duration = 5 ps , Pulse peak-power 4 kW. Power coupled to SHG crystal = 150 mW.

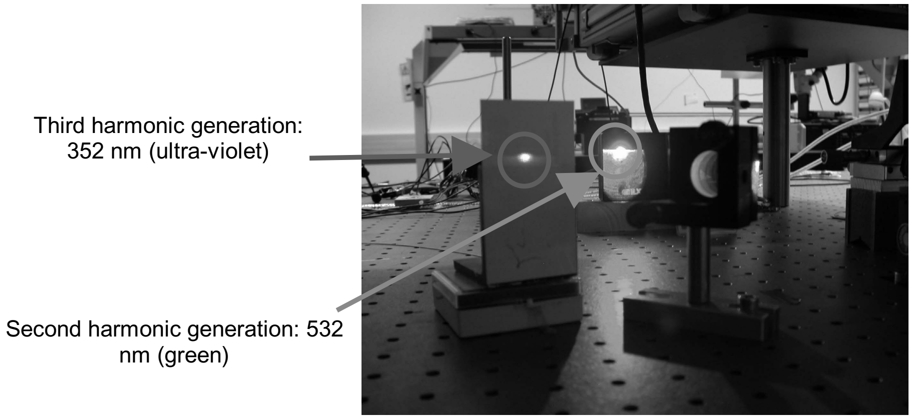

Figure 13. Frequency conversion -- second-harmonic and third-harmonic generation -- of a fibre laser.

Supercontinuum (SC) radiation generation

600 nm wide emission of 15 ps long pulses with a 1.7 W average power was demonstrated in TULE QUEST. Fig. 14 shows the schematic view of SC radiation generation using a photonic crystal fibre [16]. The pulsed beam from a mode-locked fibre laser was fed to a photonic crystal fibre, where non-linear effects took place and ended up with a broad emission band from the other end of the PC fibre. The emission spectra of two SC radiation generation experiments are shown in Fig. 16.

SC could also be generated by second-harmonic light (green) fed through a *tapered* fibre. We demonstrated a wide SC generation in the visible region by this method [17]. The schematic view and explanation of such an experiment is given in Fig. 15.

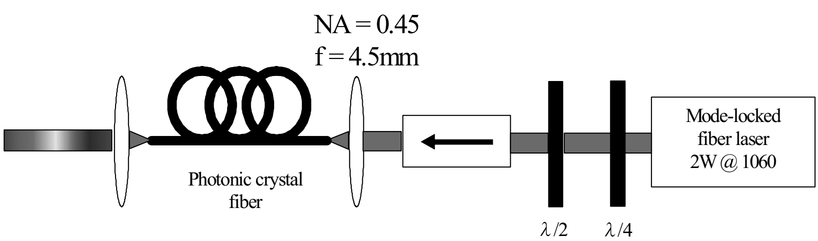

Figure 14. Schemathic view of supercontinuum radiation generation using a fibre laser and a photonic crystal fibre.

External collaboration was started with *Twente University, Netherlands*, where the recovery times of SESAMs were measured, using Twente's advanced pump-probe set-up.

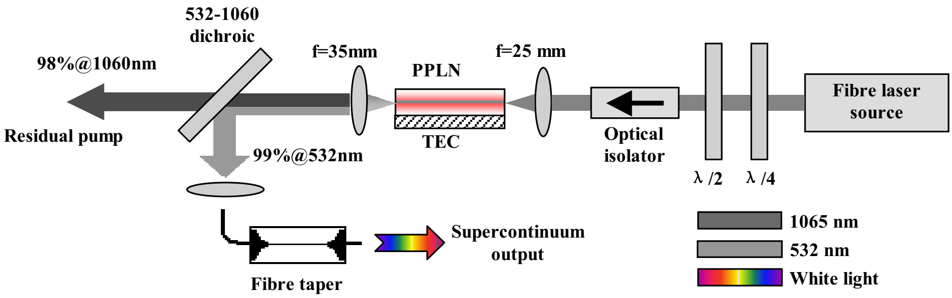

Figure 15. All-visible SC generation experiment. The fibre laser light (1060 nm) is fed to periodically-poled lithium niobate crystal to produce second harmonics (532 nm), which are led to a tapered fibre. Light intensity in the tapered fibre region was very high, and thus several non-linear effects, notably self-phase modulation and soliton formation were caused, giving rise to a broad spectrum of emitted light.

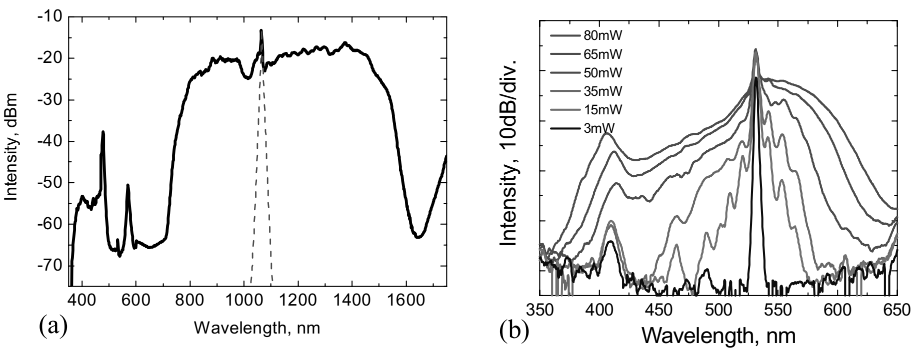

Figure 16. (a) SC radiation generation from a 1060 nm pump Yb fibre laser. The pump parameters were: average power = 2 W, pulse energy = 20 nJ, pulse duration = 5 ps, and pulse peak power = 4 kW. The parameters for the SC radiation were: pulse duration 15 ps, average power = 1.7 W, spectral width = 600 nm (5 dB bandwidth). (b) True generation of ***white light SC radiation*** from second-harmonic 532 nm light, using a tapered fibre at different input power levels. Notice the evolution of the broad spectrum at high input from a narrow spectrum at low input.

2.4 Progress Report: Progress by the Surface Science Laboratory, TUT

The work of Surface Science group in co-operation with other Partners is described in Chapter 2.2.

2.5 Progress Report: Progress by the Theory Group, TUT

The electronic structure of GaAs (110) was studied using Density Functional Theory (DFT-GGA) in atomic orbital basis (LCAO). The surface orbitals and the corresponding local density of electronic states (LDOS) were calculated to interpret experimental STM images. In interpretation, local atomic orbitals of surface atoms are related to tunnelling channels for electrons in STM imaging. The basic formalism of Tersoff-Hamann approach to STM simulation can be reformulated to reveal the role of phase difference between tunnelling channels. A destructive interference between orbitals of two neighbouring atoms increases the contrast between the two atoms, and this is reflected in directionality of STM patterns of GaAs (110) surfaces (Fig. 17).

We studied theoretically the appearance of Ga and As vacancies and antisites in X-STM images, which were taken from a *in-situ* cleaved GaAs(110) surface under different tunnelling conditions. This work helped experimentalists recognize certain features present in their cross-section STM.

We carried out electronic structure calculations on dilute GaNAs semiconductors (Fig. 18) and N interstitials in GaAs using the first-principles plane-wave pseudo-potential (PWPP) and projector augmented-wave (PAW) methods within the framework of the density functional theory (DFT). Both the ultra-soft pseudo-potential (USPP) method in connection with the generalized gradient approximation (GGA) and the PAW method in connection with the local density approximation (LDA) were employed. Effects of the single nitrogen atom and nitrogen dimer related interstitial defects on the electronic structure of GaAs were studied. Total energies, electronic band structures, and local densities of states were evaluated. In general, energies of the defects with the NN dimer at the centre of the Ga or As tetrahedron are more than 2 eV lower per nitrogen atom than the energies with a single N impurity at the same sites.

We also found that there were metastable defects with a single N impurity in the middle of a particular edge of the Ga or As tetrahedron. Second, these defect states induced drastic modifications into the electronic structure of GaAs. Interestingly, the NN dimer-related defects caused noticeable changes only to the conduction bands near the band edge, while the single N impurity-related defects modified the valence band edge. The latter also induced localized and delocalized states into the band gap. Notably, the NN dimer and N impurity defects lead to a red-shifted and blue-shift behaviour of the band gap, respectively. The observations of the blue-shift were supported by photoluminescence experiments.

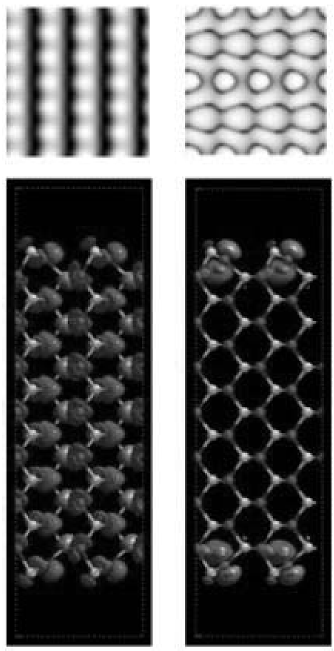

Figure 17. Supercell of the slab model for a GaAs (110) surface. One of the bulk state and surface resonance wave functions are demonstrated on the left and right, respectively. The upper panels show their contributions to the STM images.

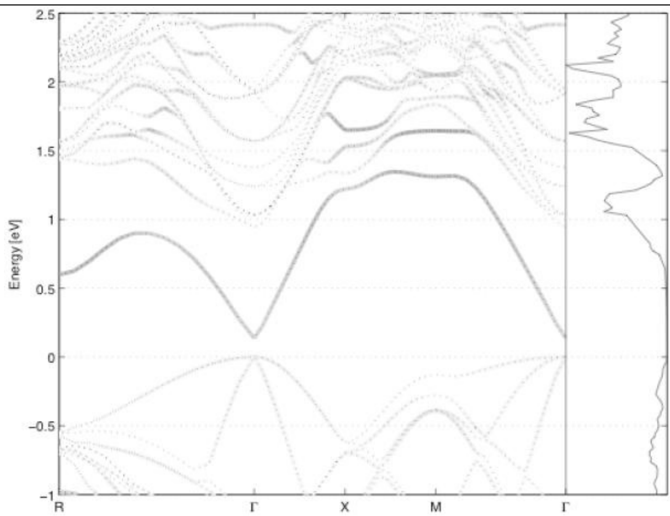

Figure 18. Calculated electronic band structure of nitrogen-doped GaAs in high-symmetry directions. The impurity contribution is pointed out with line thickness. The semiconductor “band gap problem” appearing with conventional approximations to DFT is clearly demonstrated. On the right hand, the corresponding density-of-states (DOS) is shown.

2.6 Progress Report: Progress by the Institute of Materials Chemistry, TUT

The responsibility of the Institute of Materials Chemistry for TULE QUEST was to characterize ultra-fast photo-dynamics of the QW structures and SESAMs, as described earlier in this Report (Chapter 2.2). There was a strong collaboration between ORC, IMC, UH, and the Laboratory of Physics of TUT.

The instrumentation of the femtosecond spectroscopy was extended to allow a broad tuning range of fs pulses from $\lambda = 500$ to 2000 nm. The instrument collected time-resolved absorption spectra in the visible spectrum. As an outcome of TULE QUEST a transient reflectance measurement system (pump probe) for the near-IR region (900 - 1500 nm) was built. This system was needed for direct characterization of, e.g., the dynamics of SESAMs.

2.7 Progress Report: Progress by the Laboratory of Physics, HUT

In order to understand the role of nitrogen in metastable GaInNAs alloys, positron experiments were first performed on more simple binary systems, GaN and InN. We investigated extensively the doping of GaN, and identified vacancies, either in group-III or group-V sublattices, as the dominant point defects generated by doping with Si, O, or Mg. We also investigated many different growth conditions and systems, ranging from bulk growth to different epitaxial methods. The influence on the lattice mismatch with substrate, and the interaction of vacancies and dislocations in general, were extensively studied in GaN, and recently in InN, too. We expanded similar studies to cover the semiconductors like ZnO and SiC.

Development of the positron spectroscopy was conducted. By performing experiments on Si and InP, we developed the positron methods towards studies of defect thermodynamics, such as formation energies of thermal vacancies, vacancy-impurity cluster formation, and defect migration. These studies were necessary prerequisites for the investigations of atomic clustering effects and atomic diffusion in more complex GaInNAs alloys. The operation of a pulsed positron beam was demonstrated in 2004, and this instrument was perfected in 2006. The instrument will be applied for defect identification in our future work. Other new tools prepared in TULE QUEST included a digital measurement of positron lifetime, and a low-temperature irradiation station, which was constructed for studies of radiation damage and defect kinetics. The latter was set up together with Partner P7.

2.8 Progress Report: Progress by the COMP/Laboratory of Physics, HUT

Materials properties of advanced semiconductor materials

Work on semiconductor materials and their heterostructures is in progress. COMP's basic goal was to provide understanding of the electronic and structural properties of semiconductors and structures and to see how these properties influence device performance, carrier transport etc. Point and extended defects and other growth imperfections influence the material properties. First-principles electronic structure simulations were necessary for an identification of the underlying atomistic mechanisms and proper interpretation of experimental characterization.

Materials of huge current and future interest include wide-bandgap materials, such as nitrogen based III-V semiconductors that can have various compositions, where the third-group elements can be either pure Al, Ga and In, or their combinations giving rise to various ternary and quaternary compounds. Compound semiconductors offer an excellent possibility for materials engineering and development of new materials. Variation of composition is a straightforward way for tuning the electrical and optical properties of compound semiconductor materials. We studied the electronic and structural properties, such as lattice constants, cohesive energies and band structures of the compound semiconductor alloy. Alloying included Al on Ga sublattice and As on N sublattice in various combinations.

Much of the work focused on *native defects* and *dopant-defect complexes* but we investigated also other important questions related to semiconductors. Among other things, we studied *diffusion mechanisms* for both dopant and impurity migration and self-diffusion.

We examined the electronic and structural properties, such as lattice constants, cohesive energies and band structures of GaAs and GaN -based compound semiconductor alloys in a wide concentration range. The calculations were performed using the density-functional-based code VASP (Vienna Ab-initio Simulation Package) with the projector augmented wave (PAW) method [214] and the local-density and generalized-gradient approximations (LDA, GGA). We, in particular, considered alloying with Al and In of the III-group elements and As of the V-group elements.

On the N-rich side of GaAsN strong band bowing was found, which decreased the band gap rapidly even for small changes of the composition. We also studied arsenic as a single substitutional impurity in GaN. We considered two possible substitutional sites: the Ga-site and the N-site, and found that contrary to previous theoretical results [215] arsenic preferred the N-site. The position of the As impurity level in the band gap was close to the valence band maximum in wurtzite GaN, and we believe that it could explain the near band edge emission found in many optical experiments.

Currently, one of the main topics of our research is a comprehensive study of the properties of defects, their interaction with each other and the *self-diffusion mechanisms* in GaN, AlN and Ga(Al)N. In particular, our attention was paid to modelling of vacancy-type defects in GaN, including gallium and nitrogen vacancies, di-vacancies and some larger vacancy clusters. The energies and electronic levels in the band gap were calculated for these defects in a variety of charge states. We found that in *n*-type material nitrogen vacancies can attain negative charge states up to 3-, which makes nitrogen vacancies (in appropriate charge states) the dominant self point defects for all Fermi level positions in the band gap and not only in *p*-type material, as currently assumed. Moreover, we demonstrated that the formation of mixed Ga-N di-vacancies, close vacancy pairs on the N sublattice and pairs of “oxygen-nitrogen vacancy” are favourable in terms of the energy gain.

The relatively high mobility of nitrogen vacancies in *n*-type material was demonstrated. In conjunction with the noticeable binding energies between nitrogen vacancies and other point defects, this created favourable conditions for vacancy clustering. Lattice-based kinetic Monte-Carlo simulations of vacancy diffusion at different temperatures and impurity (oxygen) concentrations demonstrated that *nitrogen vacancy clustering* can occur both homogeneously and heterogeneously (on Ga vacancies and impurities as nucleation centres), leading to the formation of small colloid Ga particles, nano-voids and oxygen nano-bubbles.

Another topic of our research that is currently in progress is the investigation of different possible dopant elements aiming to get an effective *p*-type doping of GaN, including co-doping effects. Dopant elements under consideration are individual atoms and complexes of Be, C, Si.

Electronic properties and annealing of defects in Si and Si / SiGe heterostructures

Strained Si technology enables improvements in electronic device performance and functionality *via* replacement of the bulk, cubic-crystal Si or SiGe with a Si substrate that contains a tetragonally distorted, biaxially strained Si (SiGe) thin-film at the surface. Due to changes in its crystalline structure (i.e. its symmetry is altered due to its strain state), the strained Si and SiGe film has electronic properties that are superior to those of the bulk. For example, the strained Si film has greater electron and hole mobilities, due to the change in electronic structure of the material. In this connection we performed the total energy calculations for the relaxed and biaxially strained Si and $Si_{1-x}Ge_x$ compound with Ge concentrations varied from 0 to 50 at-%:

(i) The composition dependence of atomic and electronic structure of a vacancy and di-vacancy in relaxed $Si_{1-x}Ge_x$ was calculated. These calculations were performed for random Si_xGe_{1-x} structures.

(ii) We studied the effect of strain on electronic structure of vacancy-related defects (vacancy, di-vacancy, P-vacancy complex) both in a Si layer grown on $Si_{1-x}Ge_x$ substrate and in a $Si_{1-x}Ge_x$ layer grown on a Si substrate.

Few more topics that have been studied are (i) defect-dopant interactions in doped silicon, (ii) mechanisms of defect and dopant diffusion, and (iii) effect of stress on diffusion and defect clustering.

The lattice kinetic Monte-Carlo (LKMC) simulations of vacancy diffusion in Si and Si/ $Si_{1-x}Ge_x$ /Si heterostructures have been performed in order to describe the kinetics of vacancy agglomeration into voids and vacancy-type complexes. Since the reliability of LKMC predictions is crucially sensitive to the correct assignment of vacancy jump probabilities and point defect interaction energies in different atomic environments, interatomic binding and migration energies were calculated for $Si_{1-x}Ge_x$ compounds ($0 \leq x \leq 0.5$) using density-functional theory within the generalized gradient approximation. In order to take into account the fact that $Si_{1-x}Ge_x$ heterostructures are internally strained, all defect calculations were performed assuming biaxially strained random $Si_{1-x}Ge_x$ layer grown on Si substrate. The effects of layer thickness, Ge content, spatial uniformity and external temperature on parameters of resulting structures were investigated.

Mechanism of micro crack nucleation in a highly stressed Si monocrystal

The crucial role for fracture of silicon crystallite due to its loading is played by *crack nucleation*. The crack nucleation can take place *via* different mechanisms, such as dislocation mechanism or micro crack formation by point defects. The nucleation *via* dislocation mechanism can be excluded because of the very small dislocation concentration in the silicon crystal. At the same time, application of stress to material can lead to the stress driven current of defects. This current can lead to the super saturation of defects and, therefore, result in formation of defect clusters.

Due to changes in crystalline structure (*i.e.* its symmetry is different due to its strain state), parameters that characterize diffusion current and formation of clusters, such as formation and migration energies of defects, interaction between defects can be changed significantly compare to the relaxed material and, as a result, the stress affects a cluster size and stability. In general clusters can have different shapes depending on the value and mode of loading. However, it can serve as a micro crack nucleus only provided the cluster is the planar agglomeration of point defects, which should be appropriately oriented with respect to the applied stress. Thus the main goal of the project was to acquire knowledge of whether the stress driven cluster formation can be a possible mechanism of micro crack nucleation.

2.9 Progress Report: Progress by the Accelerator Laboratory, UH

See the Chapter 2.2. The central role of Accelerator group was to perform ion irradiations for samples fabricated at ORC.

2.10 Progress Report: Progress by the Nanoscience Center, JYU

Dispersion compensating microstructure fibres were investigated regarding high-power fibre lasers [115]. Large dispersion and large mode area fibre is needed to compensate dispersion after the amplification in a fibre amplifier / laser or to compress pulses in the chirped-pulse amplification scheme. Generally, a dispersion compensating fibre has a small mode area which causes difficulties when high intensities are considered. Thus we considered a dual-core fibre geometry which was optimized with respect to large dispersion and large mode-area in order to minimize the non-linear effects. Fibre geometries with an effective mode area of 30 μm^2 with dispersion as high as -19000 ps/(nm km) and 80 μm^2 with -1600 ps/(nm km) were predicted with numerical simulations. The mode areas were larger than previously reported for dispersion compensating microstructure fibres. Also, this fibre is suitable for ultra-short pulses since the large value of dispersion has wide bandwidth.

Propagation of ultra-short pulses in erbium-doped microstructure fibre amplifiers was studied [116]. The non-linear and dispersion effects in microstructure fibres are strongly dependent on the wavelength which has to be taken into account when ultra-short pulses are considered. We included the wavelength dependence of dispersion, non-linearity, and gain into the non-linear optical Schrödinger equation, and investigated the effect on the pulse properties using numerical simulations. The pulse spectrum and chirp were shown to develop asymmetry after short propagation in the fibre amplifier. This can affect the pulse compression / dispersion compensation schemes after the amplifier. On the other hand, the wavelength dependence of non-linearity was seen to counteract the effect of dispersion, and the pulse broadening was smaller than expected.

We have also investigated waveguides in planar two-dimensional photonic crystals which could be used in integrated optical circuits. Complete decoupling between adjacent waveguides in a square-lattice photonic crystal was demonstrated for certain geometries [117]. This can be used when cross-talk between parallel waveguides in unwanted. New type of an optical waveguide realized by pattering the photonic crystal slab with a suitable material was investigated [118]. Since the band structure of a photonic crystal slab changes depending on the material on top/below the slab, the waveguide effect was shown to be due to the band gap difference of the covered and uncovered areas at some cases and due to average refractive index difference at others.

3 International Aspects

ORC

Currently, ORC is running over 20 national and international R & D projects with more than 50 Partners (universities, institutes, and companies). It is *coordinating* three EU FP6 STREP projects: *FAST ACCESS*, *URANUS*, and *NATAL* (2004 – 2007), and is a member of *EU FP5 MONOPLA* (2002 – 2006). It also acted as an EU *Marie Curie Doctoral Training Site* (2000 – 2004), which created wide international contacts. In addition, ORC belonged to European *Photonics*[21] *Network* as well as *COST 11* and *COST 288 Network*.

ORC organized international summer schools on *Optical Technologies and Applications* (under slightly varying titles every other year) in 2001, 2003, and 2005. Presently, ORC is in project collaboration with more than 50 universities and companies in Europe. The researchers were frequent speakers (invited or contributed ones) in various international conferences.

The Head of ORC, Prof. Markus Pessa, was chosen a *Member of United States National Academy of Engineering,* 2006, as the first Finnish citizen.

TCOMP/TUT

Collaboration with Prof. *Eric Larkins, University of Nott*ingham, UK: Studies of GaAs/GaInNAs interfaces recently initiated.

HUT/FYS

In the present project the researchers of the Positron Group, TUT, have had direct international collaboration with 25 institutions. The researchers of the Group gave 20 invited presentations in international conferences in 2003 – 2006. The Group participated in one EU project (CADRES) and one NORFA project (NOCDAD), which are methologically (defect analysis) directly related to TULE QUEST. The Group is currently participating in the planning of four EU FP7 projects (silicon technology, nitride optoelectronics, ZnO optoelectronics and magnetism in semiconductors). The Positron Group organized two international summer schools in the NORFA project in 2003 - 2004. Prof. Saarinen (the subproject leader until the end of 2005) was a member of four international advisory committees.

COMP/HUT

Selected collaborations

2002 – now Norway, University of Oslo, "Defects in strained Si/SiGe/Si heterostructures; computational versus experimental study."
2004 – now Norway, Institute for Microsystem Technology "Mechanism of microcrack nucleation in highly stressed Si monocrystal"

4 Publications and Academic Degrees

Table 2. Publications and academic degrees produced in Project. A list of refereed journal articles are given in Section 6.1, refereed conference papers in Section 6.2, monographs in Section 6.3, and PhD, Licentiate, and Master Theses in Section 6.4.

Partner	Type of publication	2003	2004	2005	2006	Total	Publication numbers
ORC/TUT	Ref. journal art.	1	9	10	8	**28**	**1 - 28**
	Ref. conf. papers	0	1	9	3	**13**	**119 – 131**
	Monographs	0	0	0	0	**0**	
	Doctoral dissert.	0	3	0	3	**6**	**188 – 193**
	Licentiate degrees	0	0	0	0	**0**	
	Master degrees	4	2	4	2	**12**	**176 – 187**
SURF/TUT	Ref. journal art.	0	0	0	0	**0**	
	Ref. conf. papers	0	2	0	0	**2**	**132 – 133**
	Monographs	0	0	0	0	**0**	
	Doctoral dissert.	0	0	0	0	**0**	
	Licentiate degrees	0	0	0	0	**0**	
	Master degrees	0	0	0	1	**1**	**194**
TCOMP/TUT	Ref. journal art.	0	0	2	0	**2**	**29 – 30**
	Ref. conf. papers	2	5	0	0	**0**	**134 – 140**
	Monographs	0	0	0	0	**0**	
	Doctoral dissert.	0	0	0	0	**0**	
	Licentiate degrees	0	0	0	0	**0**	
	Master degrees	0	1	1	0	**2**	**195 – 196**

IMC/TUT.	Ref. journal art.	1	2	4	5	**10**	**31 – 42**
	Ref. conf. papers	0	1	0	1	**2**	**141 – 142**
	Monographs	0	0	0	0	**0**	
	Doctoral dissert.	0	0	0	1	**1**	**197**
	Licentiate degrees	0	0	0	0	**0**	
	Master degrees	0	0	0	0	**0**	
HUT/Phys.	Ref. journal art.	12	7	10	20	**49**	**43 – 91**
	Ref. conf. papers	5	7	4	15	**31**	**143 – 173**
	Monographs	0	0	0	0	**0**	
	Doctoral dissert.	0	0	4	3	**7**	**198 – 204**
	Licentiate degrees	0	0	0	0	**0**	
	Master degrees	2	1	2	2	**7**	**205 – 211**
COMP/HUT	Ref. journal art.	0	3	4	10	**14**	**92 – 108**
	Ref. conf. papers	0	0	0	0	**0**	
	Monographs	0	0	0	1	**1**	**175**
	Doctoral dissert.	0	0	0	0	**0**	
	Licentiate degrees	0	0	0	0	**0**	
	Master degrees	0	0	0	0	**0**	
UH/Accel.	Ref. journal art.	0	0	3	3	**6**	**109 – 114**
	Ref. conf. papers	0	0	0	1	**1**	**174**
	Monographs	0	0	0	0	**0**	
	Doctoral dissert.	0	0	0	0	**0**	
	Licentiate degrees	0	0	0	0	**0**	
	Master degrees	0	0	0	1	**1**	**212**
JYU	Ref. journal art.	0	1	3	0	**4**	**115 – 118**
	Ref. conf. papers	0	0	0	0	**0**	
	Monographs	0	0	0	0	**0**	
	Doctoral dissert.	0	0	1	1	**1**	**214**
	Licentiate degrees	0	0	0	0	**0**	
	Master degrees	1	0	0	0	**1**	**213**

5 Other Activities

Since the beginning of the project, there have been *seven consortium meetings*, where the research results were presented and discussed, closely following the original schedule. Additionally, Surface Science Laboratory arranged 3 - 4 joint meetings annually with ORC, where the progress of the X-STM studies were evaluated.

COMP/HUT

International conferences:

COSIRES 2004, Finland - 7th International Conference on Computer Simulation of Radiation Effects in Solids (3 presentations of oral and poster type);
DIMAT 2004, Poland - International Conference on Diffusion in Materials (1 oral presentation);
CADRES (2004), Cicily, Italy - Workshop on Defects Relevant to Engineering Advanced Silicon-based Devices (1 oral presentation);
ICDS-23 (2005), Japan - 23nd International Conference on Defects in Semiconductors subject: (3 posters);
NSM (2005), Norway- Nordic Semiconductor Meeting (1 poster);
Psi-k meeting (2005), Germany - (2 posters);
XIth GADEST 2005, France - Gettering and Defect Engineering in Semiconductor Technology (3 oral and 1 poster presentations);
E-MRS spring meeting 2006, France - (3 oral presentations);
CADRES (2006), Grece - Workshop on Defects Relevant to Engineering Advanced Silicon-based Devices (type: oral)
E-MRS fall meeting 2006, Poland - (1 oral presentation)
Int. Workshop on Multiscale Modeling of Extended Defects and Phase Transformations at Material Interfaces 2006, Poland - (1 poster)

6 Publications

6.1 Refereed Journal Articles

P1 ORC

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CONTROLLING ELECTRONS AND PHONONS IN QUANTUM DEVICES (CODE)

Jouni Ahopelto[1] and Jukka Pekola[2].

Abstract

The goal in this project was to investigate the possibility to control electrons and phonons in nanoscale structures, targeting to development of novel devices. We have investigated the behaviour of electrons and phonons in semiconductor based structures and in normal metal-superconductor hybrid devices. Furthermore, inelastic scattering of light from confined phonons and photon heat conduction has been investigated. In the project high quality double-gated Si quantum well devices with Si channel thickness from 25 nm down to 5 nm were fabricated and characterized. The devices show volume inversion and mobility modulation effects at room temperature. At low temperatures medium thickness devices show signatures of bilayer or two-sub-band transport in conductivity and Landau level filling factor behaviour. Many-band and many-valley effects are also important in the electron-phonon heat transport. Theoretical and experimental investigation of many-band effects in carrier-phonon power loss rate was performed in this project. At very low temperatures heat is not transferred to the surroundings via the electron-phonon coupling but predominantly by electromagnetic radiation, i.e., photons. The investigations show that the heat transfer rate is limited by the universal quantum of thermal conductance. The understanding of mechanisms related to heat conduction is essential for thermal management of devices and circuits operating at very low temperatures. A thermal model is developed for Rapid Single Flux Quantum (RSFQ) control and read-out circuits and qubits. The RSFQ-qubit circuits form the basic building blocks for a quantum computer. The model is used to investigate strategies for thermal design of circuits with different power dissipation. A state-of-the-art electronic microcooler and high gain current amplifier have also been developed for ultra-low temperature electronics. As the dimensions of devices decrease, the dispersion of acoustic phonons becomes affected. The behaviour of acoustic phonons is investigated in ~30 nm thick freestanding silicon membranes at room temperature by inelastic scattering of light. Raman shifts bring out the confined phonons in these experiments. The confinement has implications for, e.g., heat transport in thin membranes. The results obtained in the project have been disseminated in 34 refereed journal articles and 26 conference presentations, including 9 invited talks. The project has produced five Doctoral and Masters thesis.

1 Partners and Funding

1.1 VTT Micro and Nanoelectronics

The research group consists of subproject leader professor Jouni Ahopelto and researchers Mika Prunnila, Leif Grönberg and Jani Kivioja.

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1.2 Low Temperature Laboratory, Helsinki University of Technology

The research group consists of subproject leader professor Jukka Pekola, senior researchers Alexander Savin and Matthias Meschke, and postgraduate student Andrey Timofeev.

1.3 Funding

The total funding for each group was 160 000 € through Academy of Finland. Besides this, about 200 000 € was spent by the LTL group on this research through the the European FP6 project "RSFQ Control of Josephson Junctions Qubits", and by the internal TKK funding.

Table 1. Funding of the project in 1000 EUR in 2003-2006. Internal funding consists of manpower costs and operational expenditures provided by the organisation. The funding provided by the Academy of Finland and other external sources is also shown in the table.

Partner	Funding organisation	2003	2004	2005	2006	**Total**
VTT	VTT	10	48	65	20	**143**
	Academy	21	61	53	25	**160**
	EU	20	0	20	0	**40**
LTL	HUT	15	26	6	3	**50**
	Academy	31	53	53	23	**160**
	Tekes	15	26	5	3	**49**
	EU			32	15	**47**
Total		**112**	**214**	**234**	**89**	**649**

2 Research Work

2.1 Objectives and Work Plan

The main objectives in this proposal are to study electron and heat transport in novel structures and devices, such as double gated quantum well structures, which can be utilized in velocity modulation transistors (VMT), and normal metal/semiconductor – superconductor hybrids. Furthermore, phononic effects and methods to control lattice heat current are explored. The VMT concept can be utilized in analogical high frequency applications at room temperature. The applications of the proposed hybrids and phononics can be found, e.g., in ultra sensitive low temperature radiation detectors and quantum computing. The work in this proposal includes fabrication and electrical, structural and thermal characterization of the solid state devices as well as theoretical investigations.

2.2 Final Report: Common Themes and Collaboration

The collaboration between VTT and LTL has been mainly concentrated on thermal and phononic effects. We have, for example, performed experimental studies of thermal electron-phonon (*e-ph*) coupling [33]. This work was initiated during the EMMA programme. Recently, we have also developed a quantitative theory that describes the *e-ph* energy transport in disordered many-valley semiconductors. When the elastic intervalley scattering time τ_{iv} dominates over diffusion the power loss P from electrons to phonons is given by [12]

$$P = S(T_e^n - T_{ph}^n), \tag{1}$$

where $T_{e(ph)}$ is the electron (phonon) temperature, n = 6 and $S \propto \tau_{iv}$. Equation 1 agrees well with experiments as can be observed from Fig. 1.

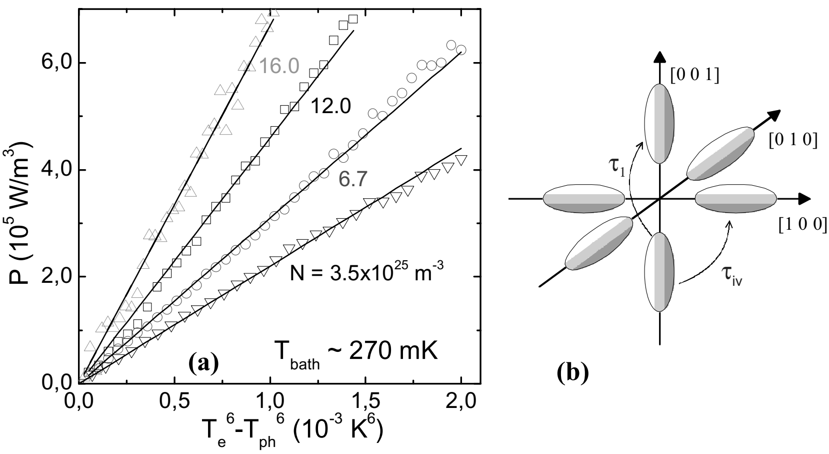

Fig. 1: (a) Experimental electron-phonon power loss in n+Si at different electron densities *N*. Solid lines are fits to Eq. (1) with τ_{iv} ~ 0.1 ps . (b) Illustration of constant energy ellipsoids of Si conduction band. Elastic scattering rate $1/\tau_{iv}$ couples the valleys which can be non-equivalent under strain field of acoustic phonon. [12]

Electron-phonon coupling plays essential role in development of Rapid Single Flux Quantum (RSFQ) circuits for sub-Kelvin applications. Weak electron-phonon coupling is a main bottleneck in cooling electrons in shunt resistors. Electron-phonon coupling strongly decreases with temperature (see Eq. (1)) and it is proportional to the volume of resistor. The volume of shunt resistor realized as a thin resistive film can be increased only up to 100–500 μm^3 without introducing harmful parasitic capacitance. Further cooling of electrons can be achieved by connecting to the resistors cooling fins with large volume and high thermal conductivity. Following these requirements new Nb trilayer process with additional 800 nm copper layer has been developed by VTT for sub Kelvin SFQ circuits and characterized [9]. The efficiency of this approach has been experimentally verified on the basic RSFQ component – balanced comparator, which is an essential part of RSFQ-based readout for superconducting qubits. In the regime where thermal fluctuations dominate over quantum effects strong dependence on temperature of the comparator uncertainty zone (gray zone) can be utilized for measurements of the electronic temperature in SFQ circuits. The width of the gray zone directly characterizes current or magnetic flux sensitivity and noise properties of SFQ circuits. Different balanced comparators fabricated with new VTT technology have been investigated during the project (fig. 2) and significant increase of comparators current resolution (40 nA at 2 GHz sampling rate) and substantial reduction of the comparator noise temperature (below 50 mK) have been demonstrated [8].

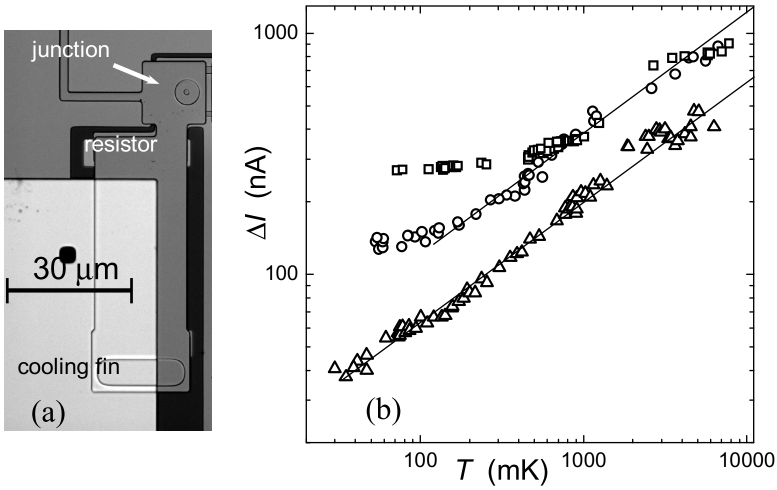

Fig. 2. (a) Optical photograph of a shunt resistor with connection to a cooling fin. (b) Temperature dependence of the gray zone for the comparator without cooling fins (critical current I_c= 2.1 µA (squares)) and for the comparators with cooling fins (I_c= 2.1 µA (circles), I_c= 0.6 µ A (triangles)). [8]

2.3 Final Report: VTT

2.3.1 Electron-phonon power loss in multi-component carrier systems

The thermal *e-ph* coupling in semiconductor systems was further studied theoretically at VTT. We explored power loss between multi-component carrier (electron) systems and phonon bath. Here the multi-component term refers to existence of carrier sub-systems, which (can) have different *e-ph* coupling constants, i.e., different *e-ph* matrix elements. One example of such system is a many-valley semiconductor where certain strain components lift the valley degeneracy. The major result here is that the inter-sub-system Coulomb interaction tends to enhance long wave length *e-ph* power loss in multi-component systems, i.e., it enhances carrier thermalization [4].

2.3.2 Phonons in thin membranes

Free-standing ~30-40 nm thick single crystalline Si membranes have been fabricated and characterized in collaboration with the groups of Prof. C. M. Sotomayor Torres and Prof. J. Groenen [23]. The membranes are fabricated on SOI substrates utilizing thermal oxidation and un-isotropic TMAH etching with oxide mask. Room temperature Raman spectra recorded from such a structure is shown in Fig. 3. The results clearly indicate the presence of confined acoustic phonons.

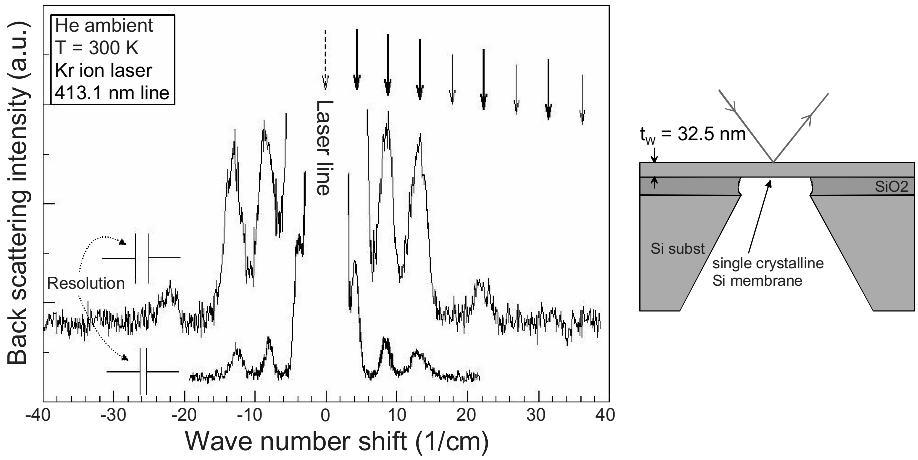

Fig. 3: Back scattering spectra of a 32.5 nm thick Si membrane and illustration of experimental configuration. The arrows indicate the expected Raman shifts due to 2D acoustic phonons. See Ref. [23] for details.

2.3.3 Transport and velocity modulation in double gated Si quantum wells

Fabrication and structural characterization (see Fig. 4) and extensive electronic transport studies of state-of-the-art single and double-gated Si quantum well FETs with well thickness t_W in the range ~ 5 – 50 nm have been performed.We have explored room temperature transport in devices with different t_W [16,21]. Experimental mobility and carrier density contours of two devices is shown in Fig. 5. The mobilities along constant carrier density contour show an enhancement towards symmetric gate bias line $V_{BG} = V_{TG}t_{BOX}/t_{OX}$. This effect is due to volume inversion/accumulation effect where the carrier distribution spreads through out the whole Si well, which is indeed the case on the basis of self-consistent distributions of Fig. 4 (c). At room temperature the total scattering rate has a minimum value at symmetric gate bias (see Refs. [16,21] and references there in).

The contour plot of Fig. 5 suggests channel current (mobility) can be modulated by adjusting the gate bias symmetry without changing the carrier density. We have reported on this experimental "intrinsic" velocity modulation [21] and Monte-Carlo study of extrinsic velocity modulation in SOI structures

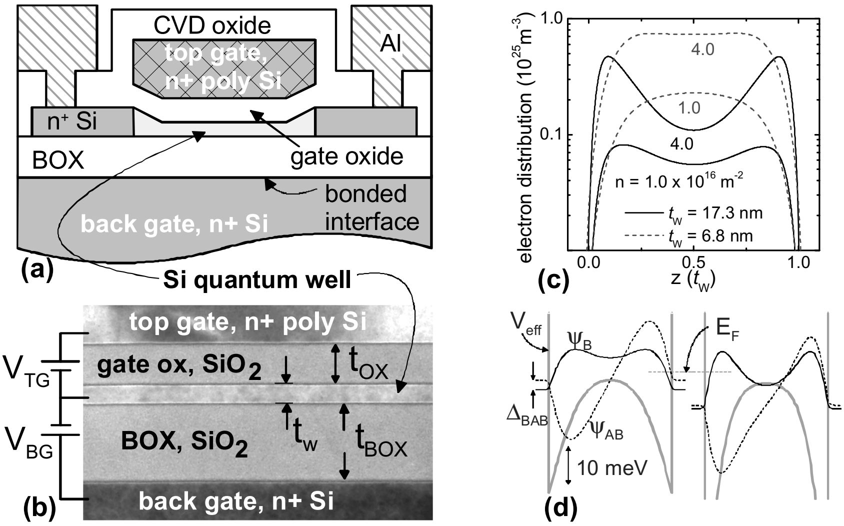

Fig. 4: (a) Schematic illustration of DG Si MOSFET cross-section. (b) TEM image of fabricated device with t_w ~18 nm and illustration of gate biasing in the transport measurements. (c) Electron distributions in the Si well at symmetric double gate bias at room temperature. (d) Formation of bonding and anti bonding states in 14 nm-thick well at low temperature. The total density n = 1E16 m^{-2} (2.8E16 m^{-2}) for the left (right) panel. After Refs. [2,16,21].

[14,17] in collaboration with the group of Prof. F. Gamiz. Furthermore, we have fabricated surface corrugated DG SOI structures, suggested by us in Refs. [17,21]. In these devices the top gate oxide-Si interface is intentionally roughened and, indeed, we have observed strong extrinsic velocity modulation effects [66]. However, the corrugation reduced the mobility in the whole channel and, thus, the total current drive.

We have performed exhaustive low temperature characterizations of the DG Si quantum wells [2,16,18] as well as single gated devices [10,27]. The best low temperature peak mobilities of VTT's DG devices are ~ 20 000 cm^2/Vs [18], which is a value comparable to high mobility bulk MOSFETs. This mobility value is high enough to make the 2D sub-bands [See Fig. 4(d)] clearly visible in the magneto transport measurements [2,18,35]. Furthermore, the zero magnetic field transport shows several interesting features due presence of many electron sub-systems. Figures 6(a) and (b) show contour plots of conductivity σ of 7 nm and 14 nm thick devices, respectively. The thinner device has only one populated sub-band [16] and shows monotonic $\sigma(V_{TG},V_{BG})$. The 14 nm-thick device has one or two sub-bands populated depending on the gate bias window and in the two-sub-band regions the conductivity shows strong non-monotonic features, which related to inter-sub-band coupling effects and sub-band delocalization (resistance resonance) [2,35]. Two-sub-band gate bias window can be detected from Fig. 6(c), which shows a gray scale plot of normalized diagonal resistivity $\rho_{xx}(B)/\rho_{xx}(B=0)$ at magnetic field of B = 2.5 T. In the single sub-band regimes the ρ_{xx} minima, related to particular Landau level filling, are continuous trajectories. When two sub-bands are occupied the trajectories are broken into a 2D interference-like pattern.

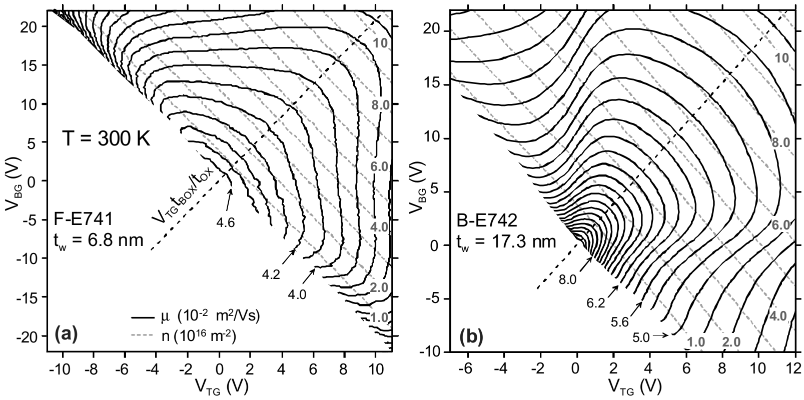

Fig. 5: Effective electron mobility μ (black thin curves) and electron density n (gray thick dashed curves with gray bold labels) as a function of top gate voltage V_{TG} and back gate voltage V_{BG} measured from (a) 6.8 nm thick and (b) 17.3 nm thick DG device at 300 K. The contour spacing for n is 1.0×10^{16} m^{-2}. For μ the spacing is 0.1 and 0.2×10^{-2} m^2/Vs in (a) and (b), respectively. The dashed diagonal line is the symmetric gate bias line $V_{BG} = V_{TG}t_{BOX}/t_{OX}$. After Refs. [16,21].

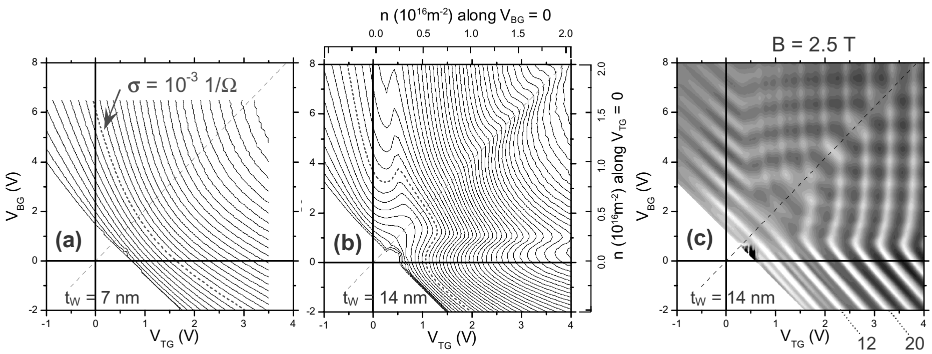

Fig. 6: Contour plot of conductivity σ as a function of top and back gate voltages measured from (a) 7 nm-thick device and (b) 14 nm-thick device. The contour spacing is 10^{-4} 1/Ω and the dashed curve is σ = 10^{-4} 1/Ω contour. (c) Normalized diagonal resistivity $\rho_{xx}(B)/\rho_{xx}(B=0)$ at B = 2.5 T. Dark and light color correspond to high and low ρ_{xx}, respectively. Two Landau level filling factors $\nu=nh/eB=12,20$ are indicated. All data measured at 270 mK. After Refs. [2,35].

2.4 Final Report: LTL

2.4.1 Electron coolers and non-equlibrium electron distribution

Thermal non-equilibrium phenomena, electron thermometry and electronic cooling in nanostructures have been investigated by LTL group within CODE project. These problems are very important for the further development of low temperature micro- and nanoelectronics [5].

Significant success in developing SINIS (superconductor–insulator–normal metal–insulator–superconductor) coolers has been achieved during the last decade in particular in LTL research group, but the limitations below 200 mK have not been fully understood yet. We suggested few mechanisms responsible for this kind of limitations, which can be used for optimization of the SINIS cooler [26,30,31]. Non-equilibrium electron distributions and the depairing density of the states within the superconducting gap were investigated in order to determine the potential of electron coolers and their ultimate performance. A state-of-the-art electronic cooler from 300 mK down to below 50 mK has been realized [26]. In addition, a novel type of efficient electron micro-refrigerator was suggested [3].

A new type of a transistor where current is controlled by electronic cooling/heating of the electron gas was realized by the LTL group [11,28]. An SEM image of the transistor is shown in Fig. 7 a. The transistor allows control of supercurrent (Fig. 7 b), which is few orders of magnitude higher than cooling current through SINIS junctions. High current gain and very low energy dissipation make this device a candidate as a current amplifier in low temperature microelectronic. Realisation of non-equilibrium electron distribution in this type of the transistor leads to significant improvement of the device characteristics [13,19,20].

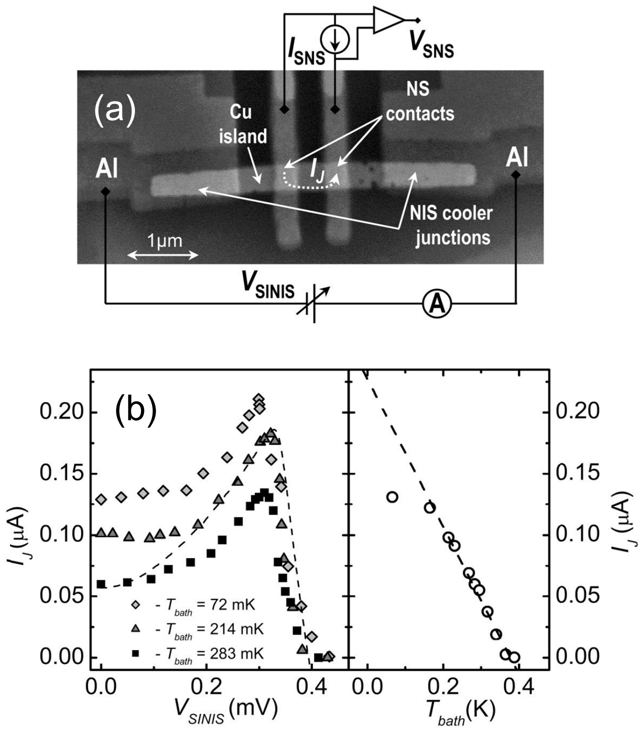

Fig. 7: SEM image of a cooler controlled superconducting Josephson transistor (a) and characteristics measured from the device (b). [28]

2.4.2. Thermal isolation in RSFQ-qubit systems

Thermal isolation and transport are important issues in microsensors and microelectronics. Self-heating due to weak coupling to the substrate can degrade the performance of the low temperature devices. Most of the important low temperature applications, such as quantum computing and thermal radiation detection are very sensitive to overheating. At sub-kelvin temperatures, when thermal conductivity of materials drops significantly and electron–phonon interaction is very weak, even a tiny power leads to significant overheating. Often the excess power dissipation of the on-chip read-out electronics can heat the systems to the limit where the benefits arising from the low temperature are lost and the device operation degrades. This problem has been investigated in case of a novel qubit (quantum bit) read-out scheme, where Rapid Single Flux Quantum electronics are used as a classical interface to multi-qubit circuits. The main aim of this part of the project is evaluation of energy dissipation and noise performance of RSFQ circuits at sub-kelvin temperatures and development of the concept of thermal design of SFQ control and read-out circuits for qubit – the basic building block of quantum computer. Partly this research was funded through the European project "RSFQ Control of Josephson Junctions Qubits".

Thermal model for RSFQ-Qubit circuits has been developed and verified experimentally [7]. Taking into account main thermal "bottlenecks" affecting operation of RSFQ-Qubit circuits we have suggested thermal design for the circuits of different complexity (power dissipation) (Fig. 8).

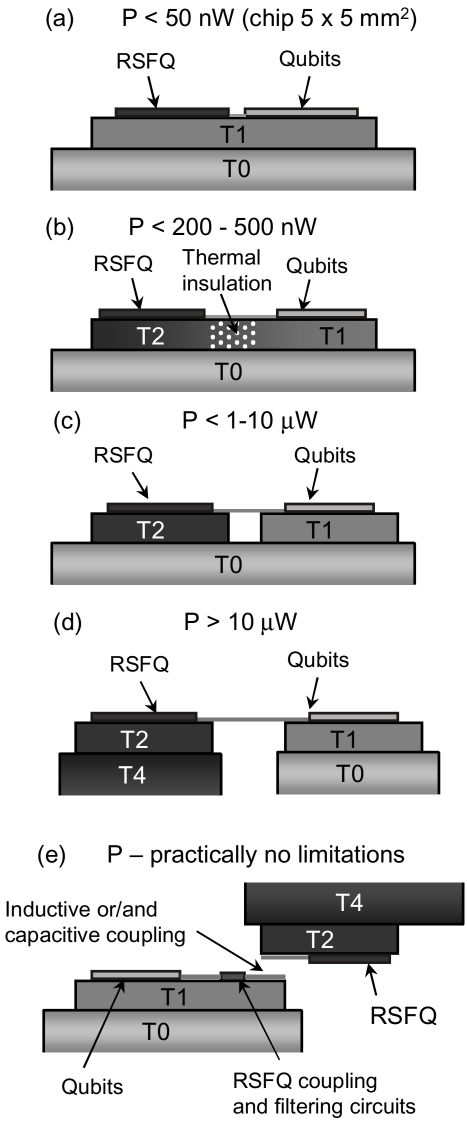

Fig. 8. Optimisation of thermal design for the circuits of different complexity. Designs with both circuits mounted at the same holder: (a) RSFQ and quantum circuits on the same Si chip, (b) substrate with improved thermal insulation between two parts, (c) two chips solution. Separate cooling of circuits with different temperatures and power dissipations: two chips with independent cooling connected by RF lines (d) and inductively (or capacitively) coupled (e). [7]

2.4.3. Quantized heat conduction by photons in mesoscopic devices

These experiments focus on heat exchange of electrons in mesoscopic devices connected to each other only via superconducting leads. Generally, superconductors are ideal insulators as regards to usual heat conduction. These new experimental results demonstrate that under certain conditions heat is not transferred via the typical electron-phonon coupling to the lattice but predominantly by electromagnetic radiation to the environment. Furthermore, these observations show that the heat transfer rate cannot have an arbitrary value but it is limited by the universal quantum of thermal conductance [1].

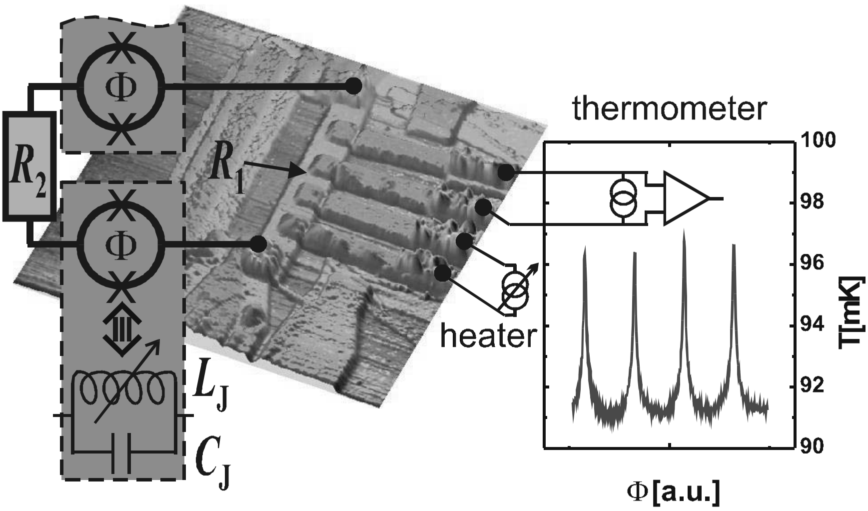

Fig. 9. Experimental setup: an atomic force microscope image (middle) of an investigated metallic island (R1) with schematic drawing (left) of the connection via superconducting lines and SQUIDs to a second, identical island (R2). Variation of external magnetic flux through the SQUIDs manipulates the coupling between both islands. R1 has in addition four NIS tunnel junctions for thermometry and additional heating. The graph (right) depicts the temperature of the electrons within R1 as a function of flux through the SQUIDs at a lattice temperature of 30mK. [1]

These experiments are directly based on earlier results of this project, as the used thermometry (SINIS thermometer) was improved within this research program (s. 2.4.1).

The observation demonstrates a very basic phenomenon, which has also consequences for new applications. The observation helps us to understand the fundamental transport mechanisms in nanoscale devices: this effect has implications for, e.g., performance and design of ultra-sensitive radiation detectors, whose operation at very low temperature is largely dependent on weak thermal coupling between the device and its environment.

3 International Aspects

VTT coordinated an assessment project EXTRA within FP5 in 2003. The activities in the project were to some extent overlapping with the workplan of CODE. Since then the collaboration with the University of Granada has continued in the field of transport in thin SOI devices. M. Prunnila spent a short period in 2004 as a visiting scientist in Granada.

VTT is also collaborating with Tyndall National Institute (former NMRC) and Paul Sabatier University on research on confined acoustic phonons in thin silicon membranes and films.

VTT has long term ties with Professor Sakaki's group at the University of Tokyo. M. Prunnila spent one month in 2004 in Prof. Sakaki's group and investigated the transport properties of double gate quantum well devices at low temperature and in high magnetic field.

LTL participates in the 6th FP project "RSFQubit" in IST, which directly relates to the present SA project. The project runs three years and it started 18.10.2004.

VTT participates FP6 project SUBTLE in IST Priority. This project started 1.10.2006. Furthermore, VTT is a member of the management board of EUROSOI coordinated action in FP6.

4 Publications and Academic Degrees

Table 2. Publications and academic degrees produced in the project. Numbers of different types of publications are given along with the reference numbers. List of refereed journal articles are given in Section 6.1, refereed conference papers in Section 6.2, monographs in Section 6.3 and theses in Section 6.4.

Partner	Type of publication	2003	2004	2005	2006	**Total**	Publication numbers
VTT	Ref. journal art.	2	5	5	5	**17**	2,4,6,8,10,12,14,16-18,21,23,27,29,30, 33,34
	Ref. conf. papers	2	4	3	3	**12**	35-37,38,39,41, 43,46-48,49,50
	Monographs	-	-	-	-	**-**	-
	Doctoral dissert.	-	-	-	-	**-**	-
	Licentiate degrees	-	-	-	-	**-**	-
	Master degrees	-	-	1	-	**1**	65
LTL	Ref. journal art.	3	10	3	7	**23**	1,3,5,7,8,9,11-13,15, 19,20,22,24-26,28-34
	Ref. conf. papers	-	3	2	1	**6**	36,40,42,44,45
	Monographs	-	-	-	-	**-**	-
	Doctoral dissert.	-	1	1	-	**2**	62,64
	Licentiate degrees	-	-	-	-	**-**	-
	Master degrees	-	-	1	-	**1**	63

5 Other Activities

Jukka Pekola organized Kilpisjärvi Spring School on Mesoscopic Physics for Graduate Students of Nordic Countries, April 30 - May 5, 2005 at Kilpisjärvi biological station (**http://ice.hut.fi/Kilpisjarvi/**)

Jukka Pekola is steering committee member of the Nanodev project at Chalmers University of Technology (http://fy.chalmers.se/nanodev/)

J. Pekola gave popular invited talks at Tieteen päivät 2005 in Helsinki (January 2005), and at Fysiikan päivät 2005 in Espoo (March 2005).

6 Publications

6.1 Refereed Journal Articles

[1] Matthias Meschke, Wiebke Guichard, and Jukka P. Pekola, Single-mode heat conduction by photons, Nature **444** (2006) 187.

[2] M. Prunnila and J. Ahopelto, "Two sub-band conductivity of Si quantum well", Physica E **32**, 281 (2006).

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[5] F. Giazotto, T.T. Heikkilä, A. Luukanen, A.M. Savin, and J.P.Pekola, Opportunities for mesoscopics in thermometry and refrigeration: Physics and applications, Rev. Mod. Phys. **78** 217 217-274 (2006) .

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6.2 Refereed Conference Papers

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[35] M. Prunnila, J.M. Kivioja, J. Ahopelto, “Double Gate Bias Dependency of Low Temperature Conductivity of SiO2-Si-SiO2 Quantum Wells”, Proceedings of the 28th International Conference on the Physics of Semiconductors, AIP Conf. Proc. (2006), in press

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6.3 Monographs

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6.4 Doctoral, Licentiate, and Master Theses

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[63] 2005 Tommi Nieminen Master Thesis on Influence of noise on Josephson junctions
[64] 2005 Jani Kivioja (June 9 2005) Doctoral Thesis on Superconducting mesoscopic electronic devices
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ELECTRONIC PROPERTIES OF CARBON NANOTUBES (ELENA)

Kai Nordlund (ACCLAB)[1], Pertti Hakonen (LTL)[2], Kimmo Kaski (LCE)[3], Esko Kauppinen (CNM) [4], Risto Nieminen (COMP)[5]

Abstract

The work in the ELENA research consortium has progressed and been finalized well. The ACCLAB and COMP groups have in close collaboration determined many of the basic properties of point defects and dopants in nanotubes. The ACCLAB and LCE groups have collaborated to examine the relation between defects and mechanical properties of the nanotubes, and in particular *shown how defects between the walls of nanotubes can strengthen them by orders or magnitude*. CNM has developed a novel aerosol and substrate chemical vapour deposition method to selectively grow SWCNT´s, based on physical vapour deposition synthesis of metallic catalyst particle aerosol prior to the CNT nucleation and growth. A new method based on nanoprobe electron diffraction to determine the chirality of individual single, double and triple walled CNT's has been developed. The CNM group has also found *an entirely new kind of carbon nanomaterial, carbon nanobuds™ , in which fullerenes and carbon nanotubes are combined in a strongly bound configuration with excellent light emission properties.* COMP has examined the effects of structural defects (vacancies, interstitials, adatoms) and dopant atoms (hydrogen, nitrogen, boron) on the electronic properties of nanostructured carbon (graphene sheets and bundles, single- and multiwalled carbon nanotubes). *The major discovery is the persistent ferromagnetism associated with structural defects, which is in many cases further enhanced by the introduction of dopants.* This discovery can have major consequences for the future applications of nanostructured carbon in spintronics device applications. The LTL group has made devices in which the shot noise of nanotubes can be measured to obtain understanding of the basic conductance properties of the nanotubes both in pristine MWNTs as well as ion irradiated ones. The results indicate that the contacts have a strong influence on the electrical conductance of the devices. LTL has also f*or the first time demonstrated gate-controlled superconductivity in carbon nanotubes.*

The ELENA consortium has created new collaborations between COMP and CNM (on simulation vs. experiments), CNM and LTL (experimental) and ACCLAB and LTL (both simulation and experimental).

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[1] Accelerator Laboratory (ACCLAB)
[2] Low temperature Laboratory (LTL)
[3] Laboratory of Computational Engineering (LCE)
[4] Center for new materials, Helsinki University of Technology (CNM)
[5] Laboratory of physics, Helsinki University of Technology (COMP)

1 Partners and Funding

1.1 Accelerator Laboratory, University of Helsinki (ACCLAB)

The research group carrying out the ELENA project consists of subproject leader professor Kai Nordlund, senior researcher Dr. Antti Kuronen, Dr. Arkady Krasheninnikov (since Jan 2005 half-time at COMP), and postgraduate students Jani Kotakoski and Niklas Juslin.

1.2 Low temperature laboratory, Helsinki University of Technology (LTL)

The research group carrying out the ELENA project consists of subproject leader professor Pertti Hakonen, senior researcher Dr. Markus Ahlskog (now professor at U. Jyväskylä), postdoc Taku Tsuneta and postgraduate students Leif Roschier, Reeta Tarkiainen and Wu Fan.

1.3 Laboratory of computational engineering, Helsinki University of Technology (LCE)

The research group consists of subproject leader academy professor Kimmo Kaski, senior researcher Dr. Antti Kuronen (since Aug 2004 at ACCLAB), postgraduate student M.Sc. (Ph.D. 2004) Maria Sammalkorpi (previously Huhtala) and student Kaisa Kautto.

1.4 Center for new materials, Helsinki University of Technology (CNM)

The research group consists of subproject professor Esko Kauppinen, Dr. Albert Nasibulin, Dr. Hua Jiang, Dr. David Brown and M. Sc. (Ph.D. 2006) Anna Moisala.

1.5 Laboratory of physics, Helsinki University of Technology (COMP)

The research group consists of subproject leader academy professor Risto Nieminen, senior researchers Dr. Adam Foster, Dr. Yuchen Ma, Dr. Arkady Krasheninnikov (before Jan 2005 at ACCLAB) and postgraduate student (PhD 2005) Petri Lehtinen.

1.3 Funding

Table 1. Funding of the project in 1000 EUR in 2003-2006. Internal funding consists of manpower costs and operational expenditures provided by the organisation. The funding provided by the Academy of Finland and other external sources is also shown in the table.

Partner	Funding Organisation	2003	2004	2005	2006	**Total**
ACCLAB	ACCLAB	30	30	30	30	**120**
	Academy	14	37	37	40	**128**
LTL	LTL	30	30	30	30	**120**
	Academy	25	42	42	23	**132**
LCE	LCE	30	30	20	20	**100**
	Academy	17	28	28	16	**89**
CNM	CNM	30	30	30	30	**120**
	Academy	25	42	42	23	**132**
COMP	HUT	20	20	20	20	**80**
	Academy	19	34	34	20	**107**
	Other	10	10	20	20	**60**
Total		**250**	**333**	**333**	**272**	**1188**

2 Research Work

2.1 Objectives and Work Plan

Carbon nanotubes (CNT's) are in many ways unique materials. A single nanotube may be only a few nanometers wide, but micrometers long, thus having an aspect ratio virtually unparalleled in any other molecule. The tubes are very strong, resilient, and stable up to high temperatures. Despite having been found as recently as 1991, they have already been subject to intense research and product development activity. They also have very interesting electronic properties and are widely regarded as a highly promising material for future electronics, offering both the possibility to manufacture conventional electronic components with properties superior to any other material, and making devices with entirely new kinds of functionality.

Basic electronic devices, such as diodes and transistors, have already been manufactured from nanotubes. However, much more research and method development needs to be performed before nanotube-based electronics reaches the level of reliability and reproducibility required for industrial electronics applications. The most significant questions to be solved include i) understanding the basic nature of electrical conductivity in nanotubes, ii) understanding what role (beneficial or detrimental) intrinsic defects and impurities have on electrical properties of nanotubes, iii) manufacturing nanotubes with suitable properties for electronics applications, and iv) designing nanotube-based electronic devices. *In this project, the consortium studied these issues with experimental and theoretical methods, and from the knowledge obtained, explored ways to manufacture devices both for conventional and superconducting electronics.*

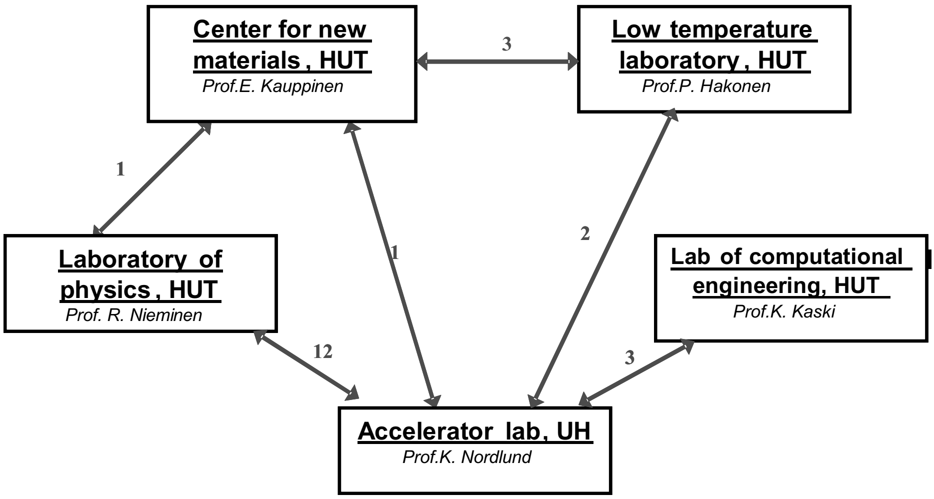

Figure 1. Realized collaborations within the ELENA consortium. The arrows and numbers indicate the number of publications which the collaborations have resulted in so far. Much additional work has been carried out between the groups, that has not yet been published.

2.2 Final Report: Common Themes and Collaboration

The ELENA project has involved extensive collaboration between the participating groups.

Collaborations within the consortium realized until now are the following. ACCLAB and LTL have collaborated on writing an overview of recent work on electrical properties of nanotubes, and are collaborating on using ion beam experiments to change electrical properties of nanotubes. ACCLAB and LCE have collaborated on mechanical properties of nanotubes. ACCLAB and CNM have collaborated on electron microscopy image simulation. ACCLAB and COMP have collaborated extensively on the topic of defect properties in carbon nanotubes. LTL has obtained nanotubes manufactured by CNM for their electrical measurements, and has begun collaboration with COMP on transport simulations of shot noise. CNM is collaborating with COMP on understanding properties of fullerenes stuck to carbon nanotubes during growth. ACCLAND and LTL have initiated collaborations on measuring the electrical properties of nanotubes *in situ* during electron irradiation. The collaborations which have resulted in joint publications are illustrated in Fig. 1.

2.3 Final Report: Accelerator Laboratory (ACCLAB)

Within the framework of the ELENA project we have continued working on the irradiation-mediated phenomena in carbon nanotubes and on effects of irradiation on their mechanical, electronic and magnetic properties. Specifically, we have addressed the annealing of the irradiation-induced defects and showed that migration of carbon adatoms (which play the role of interstitials in carbon nanotube samples) is one of the most important mechanisms of defect annealing.

We further demonstrated that the mechanical properties of multi-walled nanotubes and nanotube bundles can be improved by irradiating the tubes and suggested using small-dose electron irradiation for increasing mechanical characteristics of macroscopic nanotube products such as nanotube bucky paper and aligned ropes. The physical reason for that is irradiation-induced links between individual tubes. Although irradiation also gives rise to vacancies which lower the axial Young modulus and tensile strain of individual nanotubes, by choosing the right irradiation dose one can achieve an increase in the strength of the tube of 1-2 orders of magnitude as links between the tubes are more important.

We also showed that, similar to the conventional semiconductor technology, ion irradiation can be employed to dope nanotubes with foreign atoms and estimated the ion ranges in multi-walled nanotubes. Also, in view of growing interest in magnetic properties of all-carbon systems, we demonstrated that irradiation can give rise to magnetism in irradiated graphite and nanotube samples and thus we explained recent experimental results and opened new ways for controlling nanotube properties. We have also examined the channeling of keV energy heavy ions in nanotubes and shown that tubes can be used as nanometer-sized apertures of the ions.

In the final year of the project we developed the first Kinetic Monte Carlo simulation model for nanotubes. This code allows for simulation of defect migration in nanotubes on experimental time scales (milliseconds – minutes). The initial results show good agreement with experiments.

2.4 Final Report: Low temperature laboratory (LTL)

We have mostly investigated low frequency conductance and shot noise in MWNTs and SWNTs both in the tunneling regime as well as in quantum transport regime. The current noise measurements together with conductance can be interpreted in terms of "transmission channel fingerprints" that have been a primary analysis method in the investigations of quantum point contacts. Altogether, the noise that we measure on nanotubes is somewhat too small compared with what is expected on the basis of conductance measurements. This makes the interpretation of our results challenging and many of our works are still pending. In semiconducting samples, our results indicate that nanotube FETs are so good that they even rival SETs as the best electrometers available today. Using superconducting contacts, we have succeeded in reaching supercurrents up to 1 and 5 nA in MWNTs and SWNTs, respectively. In the latter case, we have studied the interplay of supercurrents with Fabry-Perot resonances that are visible in good quality samples. In addition, the role of disorder, either intrinsic or induced by ion beam irradiation, has been investigated in multiwalled tubes.

Semiconducting nanotube FET

A semiconducting nanotube FET was made out of a 6-nm-diameter, 4 μm long MWNT provided by the group of Sumio Iijima. We measured shot noise of this device at 4.2 K over the frequency range 600 - 950 MHz. The transconductance was found to be quite small, 3 - 3.5 μS, for optimal positive and negative source-drain voltages V. For the gate referred input voltage noise, we obtain 0.2 and 0.3 μV/Hz$^{-1/2}$ for $V > 0$ and $V < 0$, respectively. As effective charge noise this corresponds to 2 - 3 x 10^{-5} e/Hz$^{-1/2}$. It is worth to note that this charge noise is on the same order as what typical metallic SETs have.

Superconducting nanotube transistor

Superconductivity in carbon nanotubes is a complex topic. No unified picture has emerged so far from the first few investigations on this subject. We have obtained gate-controlled superconductivity in diffusive multiwalled carbon nanotubes: low frequency AC conductance was measured on a MWNT contacted using superconducting leads made of Al/Ti sandwich structure. We found proximity-induced superconductivity at 50 mK with measured critical currents up to I_{CM} = 1.3 nA, tunable by gate voltage down to 10 pA. The supercurrent branch displayed a finite zero bias resistance which varied as $R_0 \sim I^{□}$ with □ = 0.74. Using IV-characteristics of junctions with phase diffusion, a good agreement is obtained with Josephson coupling energy in the long, diffusive junction model of A.D Zaikin and G.F. Zharkov.

Noise in SWNT samples with good contacts

Our SWNT samples, made using tube material of CNM group, display a conductance pattern close to the usual Fabry-Perot pattern found in similar, good-quality samples. However, our shot noise measurements are in contradiction with the interferometric picture of non-chiral Luttinger liquids (LL). We find $F \sim 1-G/(2G_0)$, which indicates that two transmission channels are dominant in our tubes, not four as expected in the LL case. This is an indication that the degeneracy of bands is lifted by some means, presumably due to contact structure, and only two channels are contributing at the Fermi level. This result is also corroborated by the measured conductance which never exceeds 2 e^2/h in our tubes.

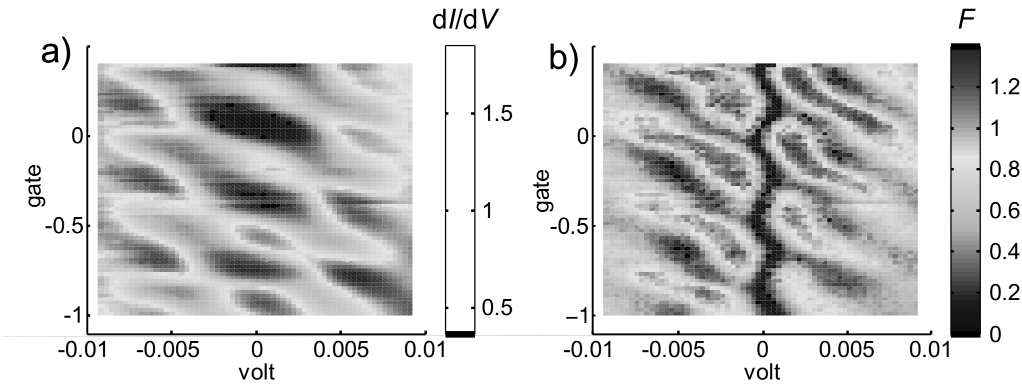

Fig. 3. (color) a) Differential conductance on the bias vs. gate voltage plane for a SWNT sample. The conductance scale on the right is given in terms of G/G_0, where $G_0 = e^2/h$ corresponds to the conductance of one quantum channel. b) Differential Fano factor. Total F and G are obtained from these results by integration along the bias axis. Measurement temperature was 4.2 K (F. Wu et al to be published).

Transport in disordered nanotubes

Very disordered, multiwalled carbon nanotubes provide good models for investigations of weak localization and interaction effects. Resistance vs. temperature measurements on catalytically grown CVD tubes, with good-quality contacts ($R_c \sim 1$ kΩ) and resistance of ~ 30 kΩ/μm, display large conductance corrections which we have analyzed in terms of the interaction effects. As a function of voltage, heating effects tend to dominate, and the dependence can be best modeled by using the equation for diffusive heat transport. The density of states of these tubes was studied using high impedance Al-AlO_x-NT contacts ($R_c \sim 100$ kΩ). We have compared our results with the theoretical calculations on tunneling into 1-dimensional disordered system, and obtained good agreement with the results beyond the first order corrections.

Local and non-local shot noise in MWNTs

We have investigated shot noise in multiterminal, diffusive (PECVD-grown) multiwalled carbon nanotubes at 4.2 K. Semiclassical theory, based on non-equilibrium distribution functions, is in agreement with our data, indicating that a major part of the noise is caused by a non-equilibrium state imposed by the contacts. Our data exhibits non-local shot noise across weakly transmitting contacts while a low-impedance contact eliminates such noise almost fully. We obtain $F \sim 0.1$ for the intrinsic Fano-factor of our MWNTs, which well below the value expected from the conductance measurements. Ion irradiation was found to reduce the measured noise, which is considered as a sign that the contacts are improved in irradiated tubes, leading to a decrease of the non-equilibrium effects. Even though these results are not understood fully from the theoretical point of view, they are nevertheless good news when considering future applications of high frequency MWNT devices.

2.5 Final Report: Progress by the Laboratory of computational engineering (LCE)

We have studied defects in nanotubes as a means to improve their mechanical properties. In multiwalled nanotubes the individual tubes interact via weak van der Waals forces, which in mechanical applications of nanotubes means poor load transfer between tubes. We have shown that intertube bonds created by e.g. electron or ion irradiation can improve the load transfer by several orders of magnitude.

Irradiation has also detrimental effects on the mechanical properties of nanotubes. Vacancy-type defects created in irradiation weaken the tubes. We have studied the effect of vacancies consisting of 1-3 missing atoms on the mechanical properties of single-walled nanotubes. Our results based on atomistic simulations and simple continuum elasticity models show that even relatively large vacancy concentrations have only a small effect on the Young's modulus of the tubes. On the other hand, the tensile strength and critical strain of the tubes may decrease by a factor of two if an unreconstructed vacancy is present. Vacancy healing by saturating the dangling bonds, however, partly alleviates the deterioration of the mechanical characteristics of the tubes.

Nanotube bundles suffer from the same weak intertube load transfer as multiwalled nanotubes. Experiments have shown that electron irradiation can be used to improve the intertube load transfer by creating intertube bonds and that there is an optimum irradiation dose below which too few bonds are created and above which the defects created in individual tubes deteriorate the mechanical properties of the bundle. We have been able to reproduce this behaviour based on a continuum elasticity model. Parameters for the model are obtained from atomistic simulations.

In addition to carbon nanotubes we have also conducted theoretical studies on hexagonal networks on closed, positively curved surfaces, such as ellipsoids. Since a perfect hexagonal lattice can not form such a surface due to geometrical limitations, it contains defects, especially disclination defects. We have studied the distribution of these defects and the effect that the surface curvature has on the distributions. We have compared the results from simulations to existing carbon networks on ellipsoids, that is, on fullerenes. The study of hexagonal lattices on curved surfaces can be used also for obtaining information on the equilibrium atomic configuration, for example, in bent carbon nanotubes.

2.6 Final Report: Progress by the Center for new materials (CNM)

A novel aerosol CVD method to elective produce SWCNT´s with selectable diameter in the range 0.8-2 nm has been developed, based on physical vapour deposition (PVD) synthesis of metallic catalyst particle aerosol prior to CNT nucleation and growth. Similar method has been developed to grown SWCNTs up to cm length via substrate CVD using catalyst particle pre-made via PVD and deposited onto substrate. A novel method based on nanoprobe electron diffraction to determine chirality of individual single, double and triple walled CNT's has been developed. Analysis of SWCNT's produced via our novel aerosol method from ethanol show that their chirality distribution is biased towards achiral tubes.

Figure 1. About 7 nm wide single-wall nanotube grown at CNM. The metal nanoparticle catalyzing the growth is visible as a black dot at the upper end of the nanotube.

The novel growth method can also lead to the growth of very wide single-wall nanotubes, see Fig. 1.

2.7 Progress Report: Progress by the Laboratory of physics, Helsinki University of Technology (COMP)

In accordance with the research plan, we have studied migration of carbon adatoms over the CNT surface, as this process may govern the supply of the “building blocks” to the growing edge (or the root) of the tube. Using density-functional plane-wave *ab initio* and tight-binding methods we showed that the adatom adsorption and migration energies strongly depend on the nanotube diameter and chirality, which makes the model of the carbon adatom on a flat graphene sheet inappropriate. Calculated migration energies for the adatoms proved to be in a good agreement with the activation energies obtained from experiments on annealing of irradiation damage in single-walled nanotubes and attributed to single carbon interstitials. The results of our atomistic simulations can readily used in macroscopic Monte-Carlo-based models of nanotube growth.

The origin of the magnetic signal reported for various carbon-based materials such as fullerenes [T. Makarova et al., Nature **413** (2001) 716] and graphite [P. Esquinazi et al. Phys. Rev. B **66** (2002) 024429] has not yet been fully understood. The magnetism in carbon systems is frequently associated with under-coordinated atoms near defects. Thus we studied the magnetic properties and the atomic structure of the most prolific defects which can appear in nanotubes or appear under irradiation: carbon adatoms, which play the role of interstitials in nanotube samples and vacancies.

After studying the fundamentals on a graphene sheet, we investigated carbon adatoms on different carbon nanotubes. We found that for every tube the energetically favored adsorption geometry is a "bridgelike" structure between two surface carbons, perpendicular to the long axis of the tube. For adsorption perpendicular or parallel to the axis, the calculations show that the adatom is spin polarized, although the magnitude of the magnetic moment depends mainly on the electronic structure of the nanotube itself.

Finally, to check the defect scenario, we modelled the magnetic properties of graphite irradiated with high-energy helium and hydrogen ions, as recent experiments [P. Esquinazi et al., Phys. Rev. Lett. **91** (2003) 227201] demonstrated that proton irradiation triggers ferromagnetism in originally non-magnetic graphite samples while He ion bombardment has a much smaller effect. We have performed spin-polarized density functional theory calculations of the magnetic properties of the defects which most likely appear under irradiation--vacancies and vacancy-hydrogen complexes. We found that both defects are magnetic. We showed that for small irradiation doses, vacancy-hydrogen complexes result in a macroscopic magnetic signal which agrees well with the experimental values. Because adsorption of H onto vacancies suppresses the annihilation of carbon interstitial-vacancy pairs, our results offer a possible explanation for the magnetic behaviour observed in the experiments.

Similar to conventional semiconductor technology, the electronic properties of nanotubes can be tailored by introducing impurities. To this end, it has been suggested to dope carbon nanotubes with B and/or N atoms. This is a natural choice of the dopant, as B/N have roughly the same atomic radius as C, while they possess one electron less/more than C, respectively.

Several methods based on arc-discharge techniques [Droppa et al. Phys. Rev. B **69** (2004) 045405, Glerup *et al.,* Chem. Phys. Lett. **387** (2004) 193] and substitutional reactions [Srivastava et al., Phys. Rev. B **69** (2004) 153414] have been developed for doping. Unfortunately, instead of occupying the substitutional sp^2 position in the graphitic network, a substantial part of the dopant is chemisorbed on the nanotube surface, forms nitrogen molecules intercalated between graphite layers, or binds to irregular carbon structures in sp^3 sites. Problems with incorporating B atoms into the carbon lattice of nanotubes have also been reported [Glerup *et al*., Chem. Phys. Lett. **387** (2004) 193]. All of these issues further limit the applicability of these techniques.

By employing atomistic computer simulations with empirical potential and density functional force models we studied B/N ion implantation onto carbon nanotubes. We simulated irradiation of single-walled nanotubes with B and N ions and show that up to 40% of the impinging ions can occupy directly the sp^2 positions in the nanotube atomic network. We further estimated the optimum ion energies for direct substitution. Ab initio simulations were used to get more insight into the structure of the typical atomic configurations which appear under the impacts of the ions. As annealing should further increase the number of sp^2 impurities due to dopant atom migration and annihilation with vacancies, we also studied migration of impurity atoms over the tube surface. Our results indicate that irradiation-mediated doping of nanotubes is a promising way to control the nanotube electronic and even mechanical properties due to impurity-stimulated cross-linking of nanotubes. We also studied magnetic properties of N impurities and showed that N adatoms on the graphite/nanotube surface have finite magnetic moments. Thus, N impurities can also contribute to the magnetism reported in carbon systems.

3 International Aspects

International meetings

The ELENA consortium arranged a joint meeting with the Swedish CARAMEL consortium also studying carbon nanotubes in August 2005, attracting about 40 participants including 3 keynote speakers from outside Finland and Sweden.

Several of the internationally best known nanotube scientists have visited ELENA groups, including Sumia Iijima (who discovered nanotubes in 1991) and David Tomanek.

LTL arranged the Kilpisjärvi Spring School on Mesoscopic Physics for Graduate Students of Nordic Countries, April 30 - May 5, 2005, with talks given by nanotube experts Herre Van der Zant, Delft University of Technology, Delft, The Netherland;

Poul-Erik Lindelöf, Niels Bohr Institute, Copenhagen, Denmark; Reinhold Egger, University of Duesseldorf, Duesseldorf, Germany.

Collaborations

All ELENA members are actively collaborating with several international groups.

ACCLAB has collaborated with Florian Banhart, University of Mainz (Germany), on irradiation and TEM analysis of nanotubes, with Steve Stuart, Clemson University (USA), on mechanical properties and with Ursula Detlaff (Germany) on properties of carbon nanotube paper. In 2006 the group initiated new collaboration with Dr. Edward Hæggström, University of Helsinki, on ultrasound measurement of carbon nanotube paper and with Prof. Roman Nowak, Helsinki University of Technology, on nanoindentation of the paper.

LTL has collaborated with and been visited by Iijima Sumio, Professor, 21 - 22.10.2004, Meijo University, Materials Science and Engineering, Nagoya, Japan; Inagaki Katsuhiko, Dr., 13 - 15.1.2005, Hokkaido University, Department of Applied Physics, Sapporo, Japan; Oda Migaku, Professor, 13 - 15.1.2005, Hokkaido University, Department of Applied Physics, Sapporo, Japan.; Strunk Christoph, Professor, 21 - 25.6.2004, Institute of Experimental and Applied Physics Institute, Departments of Physics, University of Regensburg, Regensburg, Germany; Tanda Satoshi, Professor, 13 - 15.1.2005, Hokkaido University, Department of Applied Physics, Sapporo, Japan; Tsuneta Taku, Dr., 20.6 - 20.9.2004, Hokkaido University, Department of Applied Physics, Sapporo, Japan.

CNM has the following international collaborations: Prof. David Tomanek, Michigan, State, U., USA (CNT nucleation and growth); Prof. Daniel E. Resasco, Oklahoma U., USA (CVD synthesis and chirality control); NASA Houston Labs & Rice University, Houston (chirality measurement); Prof. Juan Fernandez de la Mora, Yale, USA (HRDMA); Prof. Sergei D. Shandakov, Kemerovo State U., Russia (HRDMA theory); Dr. Peter V. Pikhitsa, Odessa Nat. Univ., Ukraine (SWCNT Nucleation)

COMP had active collaboration with the members of the CARAMEL consortium in Sweden, especially in the development of new van der Waals functionals for density-functional calculations. COMP has been visited by Dr. Youshiyuka Miyamoto, NEC, Japan (2006) and Dr. Stephen Hoffman, Univ. of Cambridge (2006).

International projects and proposals

The LTL is the coordinator in an EU STREP proposal ”Carbon Nanotube Devices at the Quantum Limit” (CARDEQ).

COMP is a partner in the EU FP6 STREP “COMP-CNT”, which is now in the final stages of negotiation with the authorities in Brussels. This project deals with the properties of carbon nanotube-polymer composites.
The CNM is partner in the 2005 - 2006 project “Investigative Support for the Elucidation of the Toxicological Impact of Nanoparticles on Human Health and the

Environment", Nanotox project (No 013908); funded by EU 6th Framework Programme on Research program;

The CNM is partner in the 2007 – 2009 project "Novel, Heteroatomic Boron, Nitrogen and Carbon Nanotubes" Project No 033350, funded by EU 6th Framework Programme on Research program.

Visits abroad

P. Hakonen, Visit Chalmers University, Gothenburg, Sweden, Group of Eleanor Campbell, 04.11.2003.

P. Hakonen, Committee member on Jaeuk Kim's Ph.D. thesis examination, Chalmers University, Gothenburg, Sweden, 26.04.2005.

Hakonen Pertti, Regensburg University, Regensburg, Germany, May 12-14, 2004. Visit to Prof. Christoph Strunk and preliminary negotiations on CARDEQ project.

Hakonen Pertti, Ecole Normale Superieure, Paris, France, Feb 6-9, 2005. Visit to Drs. Adrian Bachtold, Christian Glattli, and Bernard Placais. Negotiations on CARDEQ.

Hakonen Pertti, Ecole Normale Superieure, Paris, France, December 4-5, 2006. Visit to Drs. Adrian Bachtold, Christian Glattli, and Bernard Placais. Discussions on CARDEQ program fulfillment.

Invited and *plenary* at the following conferences:

K. Nordlund, invited talk, MRS Fall meeting, ion beam symposium, 2003, Boston, MA, USA;

K. Nordlund, invited talk, 14th International conference on Ion Beam Modification of Materials, 2004, Monterey, California, USA;

K. Nordlund, invited talk, Ion06 symposium, 2006, Copenhagen, Denmark

K. Nordlund, ICTP workshop on NanoMaterials, 2006, Trieste, Italy

A. V. Krasheninnikov, "Ion irradiation of carbon nanotubes and related phenomena", EMRS Spring Meeting, Strasbourg, France (2003).

A. V. Krasheninnikov, "Irradiation effects in carbon nanotubes", NanoteC03, Brighton, UK (2003) [selected from contributed].

A. V. Krasheninnikov, "Ion irradiation of carbon nanotubes", International Workshop on Interactions Between Nanostructures and Particle Beams, Shanghai, China, March 2004.

A. V. Krasheninnikov, "Ion irradiation as a tool to tailor properties of carbon nanotubes", CARAMEL-ELENA workshop, Helsinki, Finland, September 2004.

A. V. Krasheninnikov, “Ion irradiation of carbon nanotubes”, Nanotubes and nanostructures, Frascati, Italy, October 2004.

A. V. Krasheninnikov, "Irradiation effects in carbon systems", Advances in Functional Materials, Maroochydore, Australia, 30 Nov-02 Dec 2005.

A. V. Krasheninnikov, "Irradiation of Carbon Nanotubes: Theoretical Predictions and Experimental Results", 8th international conferences on Computer Simulation of Radiation Effects in Solids, Richland, USA, June 2006.

P. Hakonen, talk “Shot noise and electron-phonon coupling in carbon nanotubes”, NT05 conference, Gothenburg, Sweden, 26.6. - 1.7.2005.

F. Wu, T. Tsuneta, M. Paalanen, T. Wang, P. Hakonen, “Shot noise and electron-phonon coupling in carbon nanotubes”, NT05 conference, Gothenburg, Sweden, 26.6. - 1.7.2005.

R. Tarkiainen, M. Ahlskog, M. Paalanen, A. Zyuzin, and P. Hakonen, poster “Tunneling spectroscopy of disordered multiwalled carbon nanotubes”, NT05 conference, Gothenburg, Sweden, 26.6. - 1.7.2005.

Hakonen Pertti, “Single Electron Transistors: progress towards the quantum limit”, International Conference on Superlattices, Nano-structures, and Nano-devices, Istanbul, Turkey, July 30 – Aug. 4, 2006.

Lechner Lorenz “Proximity Induced Superconductivity in Multiwalled Carbon Nanotubes” VIth Rencontres du Vietnam, Hanoi, Vietnam, Aug. 6-13, 2006.

Hakonen Pertti, “Gate-controlled superconductivity in MWNTs”, March meeting of APS, Denver, USA, March 5-9, 2007.

R. Nieminen, International Workshop on *Nano-scale Materials: from Science to Technology* (Puri, India 2004).

R. Nieminen, Third International Conference on *Computational Modeling and Simulation of Materials* (Acireale, Italy 2004).

R. Nieminen, *7th Asian Workshop in Electronic Structure Calculations* (Tamkang, Taiwan 2004).

Nasibulin A. G. Fifth International Conference “Carbon: Fundamental problems, material science, technology, 12-20 October, 2006, Moscow.

Nasibulin A. G. Grenoble, France. 04 - 08 September, 2006. Congress TNT2006 "Trends in Nanotechnology".

4 Publications and Academic Degrees

Table 2. Publications and academic degrees produced in the project. Numbers of different types of publications are given along with the reference numbers. List of refereed journal articles are given in Section 6.1, refereed conference papers in Section 6.2, monographs in Section 6.3 and theses in Section 6.4.

Partner	Type of publication	2003	2004	2005	2006	**Total**	Publication numbers
ACCLAB	Ref. journal art.	-	5	6	13	**24**	1-11, 33-45
	Ref. conf. papers	-	1	-	-	**1**	C1
	Monographs	-	-	-	-	**0**	
	Doctoral dissert.	-	-	-	-	**1**	T6
	Licentiate degrees	-	-	-	-	**0**	
	Master degrees	-	1	-	-	**1**	T1
LTL	Ref. journal art.	-	5	2	3	**10**	12-18, 46-48
	Ref. conf. papers	2	-	-		**2**	C2,3
	Monographs	-	1	-		**1**	M1
	Doctoral dissert.	-	1	1		**2**	T2,3
	Licentiate degrees	-	-	-		**0**	
	Master degrees	-	-	-		**0**	
LCE	Ref. journal art.	-	3	-	-	**3**	4,7,19
	Ref. conf. papers	-	-	-	-	**0**	
	Monographs	-	-	-	-	**0**	
	Doctoral dissert.	-	1	-	-	**1**	T4
	Licentiate degrees	-	-	-	-	**0**	
	Master degrees	-	-	-	-	**0**	
CNM	Ref. journal art.	2	2	4	12	**8**	20-27, 49-61
	Ref. conf. papers	-	-	-	-	**0**	C5, C6
	Monographs	-	-	-	-	**0**	
	Doctoral dissert.	-	-	-	-	**1**	T7
	Licentiate degrees	-	-	-	-	**0**	
	Master degrees	-	-	-	-	**0**	

COMP	Ref. journal art.	1	5	1	-	**7**	1, 2, 10, 29-32
	Ref. conf. papers	-	-	-	-	**0**	
	Monographs	-	-	-	-	**0**	
	Doctoral dissert.	-	-	1	-	**1**	T5
	Licentiate degrees	-	-	-	-	**0**	
	Master degrees	-	-	-	-	**0**	

5 Other Activities

The ELENA consortium has arranged 4 half-day meetings of the whole consortium, and the joint ELENA-CARAMEL meeting mentioned above.

The results have been disseminated to the wider public in an article in Prosessori-lehti (Nov 2004 and Feb 2007 issues) written by P. Hakonen and E. Kauppinen and K. Nordlund [O1] as well as by P. Hakonen, L. Lechner and M.Tomi [O2].

The CNM group (Esko Kauppinen) have developed and applied for patents for new nanotube production method [P1-P4].

6 Publications

6.1 Refereed Journal Articles

[1] A. V. Krasheninnikov, K. Nordlund, P. Lehtinen, A. S. Foster, A. Ayuela, and R. M. Nieminen, Adsorption and migration of carbon adatoms on zigzag carbon nanotubes, Carbon 42, (2004).
[2] A. V. Krasheninnikov, K. Nordlund, P. O. Lehtinen, A. S. Foster, A. Ayuela, and R. M. Nieminen, Adsorption and migration of carbon adatoms on carbon nanotubes, Phys. Rev. B 69, 073402 (2004).
[3] J. A. V. Pomoell, A. V. Krasheninnikov, K. Nordlund, and J. Keinonen, Ion ranges and irradiation-induced defects in multi-walled carbon nanotubes, J. Appl. Phys. 96, 2864 (2004).
[4] M. Sammalkorpi, A. Krasheninnikov, A. Kuronen, K. Nordlund, and K. Kaski, Mechanical properties of carbon nanotubes with vacancy-like defects, Phys. Rev. B 70, 245416 (2004), see also Erratum.
[5] J. A. Åström, A. V. Krasheninnikov, and K. Nordlund, Carbon nanotube mats and fibers with irradiation-improved mechanical characteristics: a theoretical model, Phys. Rev. Lett. 93, 215503 (2004), also selected to Virtual Journal of Nanoscale Science & Technology Vol. 10 Issue 22 (2004). See also Erratum.
[6] J. Kotakoski, J. Pomoell, A. V. Krasheninnikov, and K. Nordlund, Irradiation-induced substitution of carbon atoms with nitrogen and boron in single-walled carbon nanotubes, Nucl. Instr. Meth. Phys. Res. B 228, 31 (2005).
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[31].Magnetic properties of vacancies in graphene and single-walled carbon nanotubes - Y. Ma, P. O. Lehtinen, A. S. Foster and R. M. Nieminen N. J. Phys. 6 (2004) 68
[32] Irradiation-induced magnetism in graphite: a density-functional study - P. O. Lehtinen, A. S. Foster, Yuchen Ma, A. V. Krasheninnikov and R. M. Nieminen Phys. Rev. Lett 93 (2004) 187202
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6.2 Refereed Conference Papers

[C1] K. Nordlund, J. Nord, A. V. Krasheninnikov, and K. Albe, Atomic-scale simulations of radiation effects in GaN and carbon nanotubes, in Radiation Effects and Ion Beam Modification of Materials, Vol. 792 of MRS Symposium Proceedings, edited by L. M. Wang, R. Fromknecht, L. L. Snead, D. F. Downey, and H. Takahashi (MRS, Warrendale, PA, USA, 2004), p. 531.
[C2] R. Tarkiainen, M. Ahlskog, P. Hakonen and M. Paalanen, Electron heating effects in disordered carbon nanotubes, J. Phys Soc. Jpn. 72 Suppl. A, 100 - 101 (2003).
[C3] R. Tarkiainen, M. Ahlskog, P. Hakonen, M. Paalanen, Transport in disordered carbon nanotubes, Physica E 18, 206 -207 (2003).
[C4] Tolochko, O. V., Nasibulin, A. G. Choi, C.-J., Altman, I., Kim, B.-K. and Kauppinen, E. I. Aerosol synthesis of iron and iron carbide nanoparticles: experimental and theoretical study, Abstracts of the 2003 European Aerosol Conference, Mardid, Spain, 31 August - 5 September, 2003. *J. Aerosol Sci.* V.1. 301-302.
[C5] Shandakov, S. D., Nasibulin, A. G., Kauppinen, E. I. Electrical mobility of particles in nano- and sub nanometer range: review and a new approach, Abstracts of the 2003 European Aerosol Conference, Mardid, Spain, 31 August - 5 September, 2003. *J. Aerosol Sci.* V.2. 927-928.
[C6] Nasibulin, A. G., Moisala, A., Brown, D. P., Kauppinen, E. I. (2003) Aerosol production of carbon nanotubes and onion particles, Abstracts of the 2003 European Aerosol Conference, Mardid, Spain, 31 August - 5 September, 2003. *J. Aerosol Sci.* V.1. 103-104.

6.3 Monographs

[M1] M. Ahlskog, C. Laurent, M. Baxendale, and M. Huhtala, “Electronic properties and applications of carbon nanotubes”, in F. Nalwa (ed.), Encyclopedia of Nanoscience and Nanotechnology, 2004 pp. 139-161.
[M2] Ch. 16, The magnetic nature of intrinsic and irradiation-induced defects in carbon systems' *P. O. Lehtinen, A. V. Krasheninnikov, A. S. Foster and R. M. Nieminen* in 'Carbon-Based Magnetism *T. Makarova and F. Palacio eds.* Elsevier, North-Holland (2006)

6.4 Doctoral, Licentiate, and Master Theses

[T1] Jani Kotakoski, Master’s thesis, University of Helsinki 2004.
[T2] L. Roshier, “Carbon Nanotube Single-Electron Devices at Audio and Radio Frequencies”, Ph.D. thesis, Helsinki University of Technology, 2004, ISBN 951-22-7096-X.
[T3] R. Tarkiainen, “Transport and Tunneling in Multiwalled Carbon Nanotubes”, Ph.D. thesis, Helsinki University of Technology, 2005, ISBN 951-22-7700-X.
[T4] M. Sammalkorpi, Molecular Dynamics Simulations of Strained and Defective Carbon Nanotubes, Ph.D. thesis, Helsinki University of Technology, 2004.
[T5] P. Lehtinen, Magnetic Nature of Intrinsic Carbon Defects, Dr.Sc.(Tech.) dissertation 129, Laboratory of Physics, Helsinki University of Technology, 2005.

[T6] J. Kotakoski, "Irradiation-induced tailoring of carbon nanotubes", Ph.D. thesis, University of Helsinki, 2007
[T7] Anna Moisala "Studies on synthesis of single-walled carbon nanotubes by gas-phase chemical vapour deposition" PhD dissertation, 3rd of March, 2006. Helsinki University of Technology.

7 Other References

Invited overview articles

[I1] K. Nordlund and P. Hakonen, *Nanotubes - Controlling conductance*, Nature Materials **4**, 514 (2005).

Publications popularizing science

[O1] P. Hakonen, E. Kauppinen, and K. Nordlund, Atomitason elektroniikkaa, Prosessori, November 2004, 32-34.

[O2] P. Hakonen, L. Lechner, ja M. Tomi, *Nanoputket vipisevät*, Prosessori, February 2007.

Patents

[P1] A. G. Nasibulin, E. I. Kauppinen, D. P. Brown, A. Moisala (2005) Carbon onion particle synthesis. (filed on June 4, 2003). FI 20035120.

[P2] A. G. Nasibulin, E. I. Kauppinen, D. P. Brown, A. Moisala, H. Jiang (2005) Carbon nanotubes and composites of carbon nanotubes with controlled properties, a method to produce said carbon nanotubes, functional matrix and composite materials composed thereof and structures and devices fabricated from the same. (filed on March 9, 2004). WO 2005085130.

[P3] A. G. Nasibulin, D. P. Brown, H. Jiang, E. I. Kauppinen, (2005) Fullerene covalently functionalized carbon nanotubes, a method and apparatus to produce them and composites thereof. (filed on November 16, 2004).

[P4] Kauppinen, E.I., Gonzales, D., Nasibulin, A.G., Brown, D.P. (2006) Method for moving High Aspect Ratio Molecular Structures. Patent Application, Submitted, March 2006.

LOW POWER BIOMORPHIC NEURAL CIRCUITS BASED ON FLOATING GATE MOS AND SET TRANSISTORS

Project manager: Prof. Jukka Tulkki. Helsinki University of Technology Laboratory of Computational Engineering (LCE)
Subproject leaders: Prof. Kari Halonen, Helsinki University of Technology Laboratory of Circuit Design (ECDL), Prof. Markku Åberg, VTT Information Technology/Microelectronics (VTT) and Helsinki University of Technology Laboratory of Circuit Design (ECDL), Prof. Matti Weckström, (University of Oulu) Biophysics Laboratory (OY)

LCE:
Teknillinen korkeakoulu
Laskennallisen tekniikan laboratorio
PL 9203
FIN-02015 TKK
ECDL:
Piiritekniikan laboratorio
PL 3000
02015 TKK
VTT:
VTT Tietotekniikka
PL 1200
02044 VTT
OY:
PL 3000
90014 Oulun yliopisto

Abstract

The project goal is to develop a fast, power and area efficient multiple input floating gate transistor based neural circuit structures for signal processing. These transistors can perform combined operations - summing, multiplication - on a single transistor. The floating gate transistors can be realised either with MOS technology or nanotechnology devices, like SET (Single Electron Transistor) transistors. The goal of the project is to develop power optimised neural structures, based on the ideas taken from extremely energy efficient biological neurons, to develop SET devices and their models, especially integration capability in mind, and finally to combine them into SET based neural circuit structures.

1 Partners and Funding

1.1 Laboratory of Computational Engineering, Helsinki University of Technology

The research group consists of project leader professor Jukka Tulkki and postgraduate students MSc Teppo Häyrynen, MSc Roman Terechonkov.

1.2 Electronic Circuit Design Laboratory, Helsinki University of Technology

The research group consists of subproject leader professor Kari Halonen and postgraduate student Jacek Flak.

1.3 Integrated System Circuits, VTT

The research group consists of project leader professor Markku Åberg, MSc Arto Rantala, MSc Jan Saijets and Mr. Jani Mäkipää (design), Prof. Jouni Ahopelto, MSc Mika Prunila, MSc Jani Kivioja and Ms. Eeva-Riitta Pursula (process and SET measurements).

1.4 Biophysics division and laboratory, Department of Physical Sciences, Univ. of Oulu

The research group consists of subproject leader professor Matti Weckström, senior researcher Dr. Stephan Krause, Dr. Mikko Vähäsöyrinki (presently in California Institute of Technology), postgraduate students Lic.Sci Kyösti Heimonen, Lic.Sci. Mika Kauranen.

1.5 Funding

Table 1. Funding of the project in 1000 EUR in 2003-2006. Internal funding consists of manpower costs and operational expenditures provided by the organisation. The funding provided by the Academy of Finland and other external sources is also shown in the table.

Partner	Funding organisation	2003	2004	2005	2006	**Total**
LCE	HUT	20	20	20	20	**80**
LCE	Academy	15	30	30	14	**89**
ECDL	Academy	14	38	52	28	**132**
VTT	VTT	40	62	62	30	**194**
VTT	Academy	24	61	61	31	**177**
OY	OY	75	75	80	80	**310**
OY	Academy	0	25	25	25	**75**
Total Academy		**53**	**154**	**168**	**98**	**473**
Total		**188**	**311**	**330**	**228**	**1057**

2 Research Work

2.1 Objectives and Work Plan

The neural circuits based on floating gate transistors are one of the most promising ways to implement fast and low power circuits with high computational capacity. The principle of floating gate transistors and neural processing with them can be expanded beyond CMOS technology. Takahashi & al [Y. Takahashi, Y. Ono, A. Fujiwara & H. Inokawa, “Silicon Single-Electron Devices for Logic Applications”, Proc. Of the ESSDERC 2002, pp. 61 – 68.] have presented the possibility to adapt the neuro-MOS computing principle to SET.

The power and computational efficiency come from the following facts:

1. A single transistor with a gate capacitor array performs complex operations, like multiplication or simultaneous summation of several signals. With SETs a XOR gate with a single transistor and multiple gates is possible.
2. The operation is highly parallel. At least forty parallel inputs can be connected to a single neuro-MOS.
3. The input processing is capacitive. Power consuming dc-bias is needed only for the output.

The noise tolerant neural approach is considered as the most promising for SETs because A: it is very difficult to make a matched pair of SETs, thus excluding standard analog approach; and B: it is very difficult to adjust the switching points of SET based standard logic gates, thus excluding standard digital approach in signal processing.

In this project neuro-MOS and neuro-SET based neural networks are developed and studied, especially for fast and power efficient signal processing. Neuro-MOS structures, including MOS capacitor based, and neuro-SET structures, are studied and optimized in deep sub-micron line width processes. Power optimisation will be studied, based on physical and architectual ideas from extremely power-efficient biological neurons. New efficient algorithms utilizing the benefits of neuro-structures are developed. Models for simulation of neuro-SET structures are developed. The applicability of floating gate structures – either MOS or SET – to higher level neural architectures, e.g. recurrent or CNN, will be studied.

<u>Tasks</u>

1. Study of energy efficiency of biological neurons and implementation of the biological energy saving means to electronic circuits

The means for achieving the extremely low power consumption in biological neurons will be studied. Preliminary research indicates that they utilize e.g. massive parallelism, spread information transmission, analog signal processing and level restoring by digitalization.

2. Neuro-SET structures

Multi gate SET transistors suitable for floating gate principle neuro computing will be developed, processed and characterisised. Circuit simulation models for them will be developed and demonstrator neuro-SET circuit blocks will be made.

3. *Optimal neuro-circuit topologies in main neural architectures.*

Generic neuro-MOS or SET computational circuit blocks will be developed and studied with different architectures. These can include e.g. CNN (cellular neural network), feedforward or recurrent circuits.

4. *Models and simulation strategies*

Neuro-circuits are basically analog circuits that are doing complex, not necessarily periodic computational operations. Therefore the circuits should be simulated in transient analog mode. New simulation models must be developed for SETs.

5. *Applications and demonstration circuits*

Demonstration circuits oriented to telecommunications applications will be designed and processed.

6. *All optical processors and circuits for biomorphic image processing*

This is a new research topic that was added during the research period. It aims at developing all optical signal processors. One subfield of potential applications are biomorphic optical circuits.

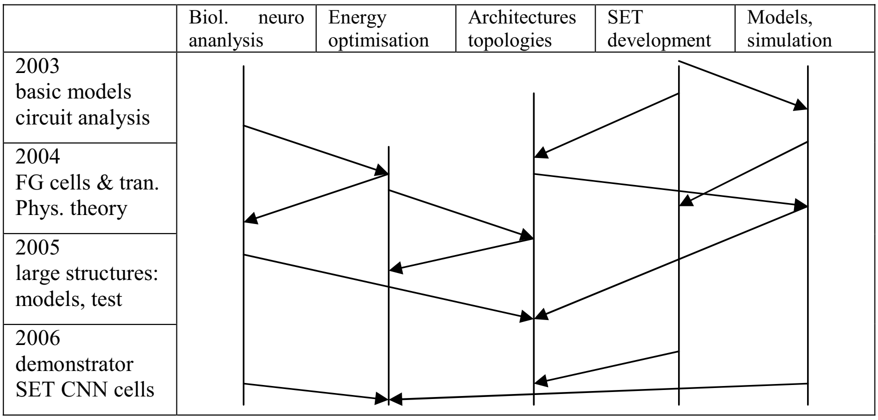

Figure 2.1.1. Project flow and the links between the tasks

2.2 Final Report: Common Themes and Collaboration

The goal of the project proposal has been to integrate of nano- and bio-technologies for future ICT applications. The separate projects have proceeded as planned but the integration of nanoelectronic and bioscience is still being worked out at conceptual level. However, it was well known *a priori* that recognising and understanding of the structural and functional differences in electronic SET and biomolecular information systems is challenging and time taking process. We believe that we are able to make good progress in the integration of knowledge in the near future.

2.3 Laboratory of Computational Engineering, Helsinki University of Technology

The work done has focused on studying the biophysical properties and the intercellular signalling of neurons. So far we have studied existing neuron models and tried to develop an electrical equivalent circuit model that could reproduce the behaviour of the neurons. In addition work has been done on basic structural and transport properties of compound and silicon structures to evaluate their potential in biomorphic networks.[2] At the moment we are also working on modelling of multigate SOI based SET fabricated by VTT Information technology Centre for Microelectronics, see below. During the project a new research topic of optical processors has been added to research plan. The basic building block of all optical circuits is a bistable system of two phase locked lasers.[3-5] The advantage of the flip-flop memory shown schematically in Fig. I1 is that the both lasers are above threshold and therefore the operation is not delayed by the switching the lasers across threshold. Bistable laser configurations similar to those represented in Fig. 2.3.1 can be used to greate all optical logic gates.[5]. This work is part of the doctoral thesis of Jani Oksanen[D2]. We have proposed a biomorphic circuit that would make use of these components and mimic the operation of the compound eye in detecting weak light signals.

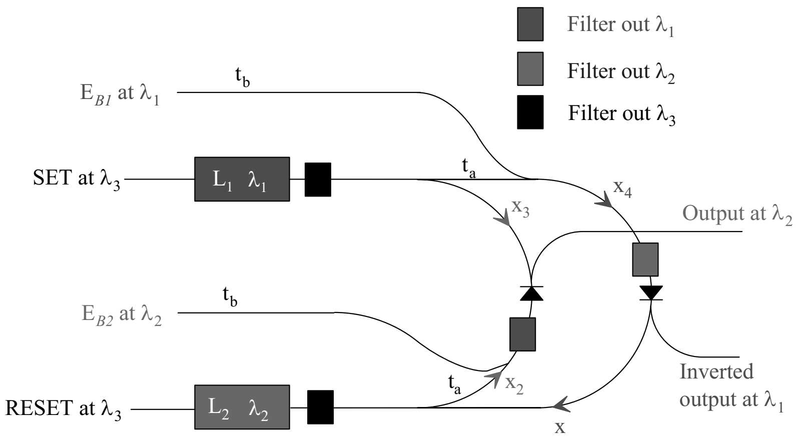

Figure 2.3.1. A schematic representation of a coherent optical flip-flop[3]. The flip-flop can operate as a fast memory unit and composes of phase locked laser amplifiers, antireflectors (or optical isolators) and interferometers. With minor modifications the structure is also capable of performing logical functions and signal regeneration operations. The operation of the device is based on the nonlinear coupling of two laser amplifiers, which form a bistable system. The nonlinearity originates from the interference of coherent optical signals. The two stable states of the bistable laser system form the two states of the memory. The states of the flip-flop can be set (reset) by sending an optical pulse into the set- (reset-) port of the device, and the state of the memory can be read from the output port.

2.4 Electronic Circuit Design Laboratory, Helsinki University of Technology

This part of the project was focused on the development of circuit structures inspired by the biological systems, which are suitable for implementation with floating gate MOS (FG-MOS) and single-electron tunneling (SET) transistor. The design efforts were put to take the full advantage of the extended functionality found in the floating gate devices. The subproject has been conducted in two parallel ways. On one side, the existing expertise in cellular neural/nonlinear network (CNN) technology and its CMOS implementation have been extended and as a result, the complete binary-programming scheme has been established. In this way, the cellular array processor can robustly be provided versatility at the minimum hardware expense. On the other side, a new binary CNN architecture with cells utilizing the FG-MOS structure were developed as a step towards a CNN implementation with nanotechnology. Based on the knowledge gained from this design, a new programmable CNN cell has been built with SET transistors.
Obtaining a massively parallel (brain-like) computing with integrated circuits is both appealing and challenging task. CNN [CY1998] with its enormous computing power is the most promising approach to many high-speed image and video processing. It is also considered as one of the best approaches to development of systems based on nanodevices. CNN is an array of identical processing elements (locally interconnected) performing the same global instruction on their own local data. Therefore, it can be classified as a single-instruction multiple-data (SIMD) type processor.

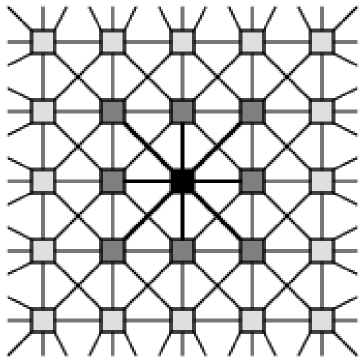

Figure 2.4.1. Typical cell arrangement and interconnections in CNN array: rectangular grid with fully connected 1st order neighborhood.

CNN architecture is naturally suitable for image processing with each cell corresponding to a pixel of an image. The network behavior can conveniently be described with the cell state equation:

$$\frac{dx_{i,j}(t)}{dt} = -x_{i,j} + \sum_{k,l} A_{k,l} \cdot y_{k,l} + \sum_{k,l} B_{k,l} \cdot u_{k,l} + I \qquad (2.4.1)$$

where: $\boldsymbol{x_{i,j}}$ is the state of a cell at ***i***-th row and ***j***-th column of the array, ***k*** and ***l*** are the neighborhood co-ordinates, ***A*** is a matrix containing feedback template coefficients, ***B*** is a template matrix with feedforward coefficients, ***y*** is the network output, ***u*** is the network input, and ***I*** is the threshold term. In general, both the cell state and the coefficients can be real values. A special subclass is binary CNN that can operate on black-and-white (B/W) images only. It is a very important class covering a wide range of operations [CNN-SL]. When the network is dedicated for B/W image processing, the cell state and coefficients can be reduced to binary values. In this way, the programming becomes digital, and thus fast and robust. Moreover, the two template matrices can be replaced by one matrix containing elements of either one of them, and the type of operation is then selected with a digital control signal. The threshold ***I*** is 2-bit programmable to 0.5, 1.5, 2.5, or 3.5. Due to all these changes, the more complex operations are performed algorithmically as a sequence of simple subtasks.

The developed CNN cells arose from the basic neuron model proposed by McCulloch and Pitts, presented in Fig.2.4.2, and evolved into more advanced structures. Although this model does not reflect the current status of the knowledge, it is often referred to, since it allows for simple representation of the basic neuron functionality. The multiple input signals are multiplied by the corresponding synaptic weights and then summed. The result and the threshold value are fed to the limiter, which shapes the output signal according to the activation function. In principle, the threshold value ***S*** can be threaten as another input signal (with opposite polarity). In the presented design, the activation function has a form of a step function.

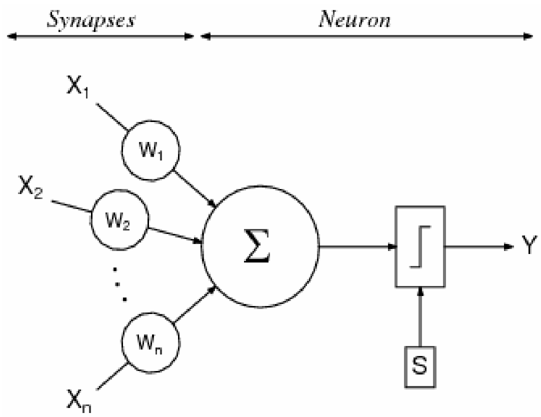

Figure 2.4.2. The neuron model by McCulloch and Pitts.

The idea of floating gate MOS structure (also known as "neuron MOS") has been proposed by Shibata and Ohmi [SO1992] and immediately gathered attention as very suitable for building neural circuits. The structure and its electrical model are presented in Fig.2.4.3. Such a device is able to perform a weighted voltage-mode sum and threshold operations. The potential of the floating gate is set by the input voltage weighed by the values of coupling capacitors, and can be written as:

$$\Phi_F = \frac{\sum_{i=0}^{n} C_i V_{in\_i}}{\sum_{i=0}^{n} C_i} \quad (2.4.2)$$

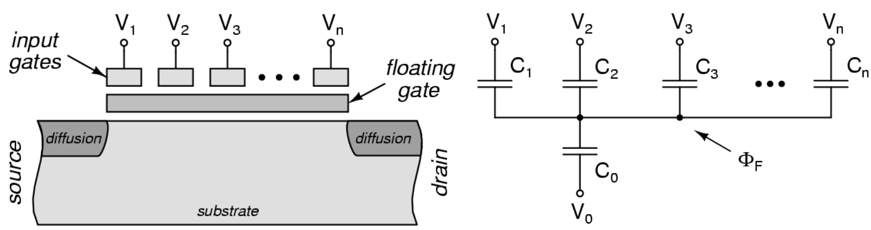

Fig. 2.4.3. The sketch of the neuron MOS structure and the corresponding electrical model. $\mathbf{C_0}$ represents the substrate parasitic capacitance.

An interesting and useful is the floating-gate CMOS inverter resulting from the complementary combination of N- and P-type devices. This simple circuit (shown schematically in Fig.2.4.4.) implements all the functionality described by the McCulloch and Pitts neuron model.

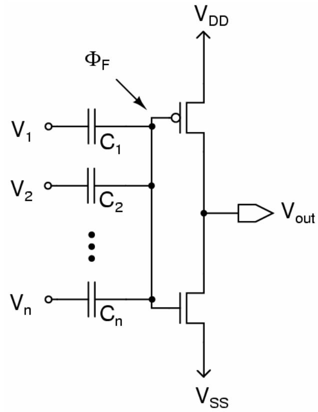

Figure 2.4.4. The floating-gate CMOS inverter schematic

Based on the floating gate CMOS inverter structure, the CNN cell has been developed. Its structure is shown in Fig.2.4.5. Nine synapses with 1-bit programmability connect a neuron to its neighborhood. Each synapse consists of a unit capacitor and two switches. Template coefficient, $\boldsymbol{AB_i}$, and the output of the respective neighbor, $\boldsymbol{V_{Yi}}$, control the switch transistors. When both switches conduct, the synapse is active and the floating node is coupled through the unit capacitance to the supply voltage, $\boldsymbol{V_{DD}}$. The 2-bit programmable threshold is set by the bias circuit, which has a form of additional three synapses with capacitances scaled with respect to the unit capacitor. Additionally, the synaptic circuits of the bias couple the floating node to the ground, $\boldsymbol{V_{SS}}$, instead of $\boldsymbol{V_{DD}}$. In this way an opposite influence on this node potential is obtained. A summation is performed via charge redistribution in the capacitive network at the pseudo floating gate, and the result is fed to the cascade of inverters that shape the nonlinear output function. When the number of active synapses exceeds the programmed threshold value the neuron triggers. The transient mask structure and additional switches are required for logic functions and more complex operations that require a fixed state map. The block of local memories is used to store the intermediate results during algorithm evaluation. With all these extensions, the designed neuron becomes a complete and very versatile CNN cell. At the same time, the area efficient implementation is possible. Simulated neuron activation at different bias values is shown in Fig.2.4.6. A number of network operations were tested, and the selected results are shown in Fig.2.4.7. More details about the cell functionality and design issues can be found in Reference [C4].

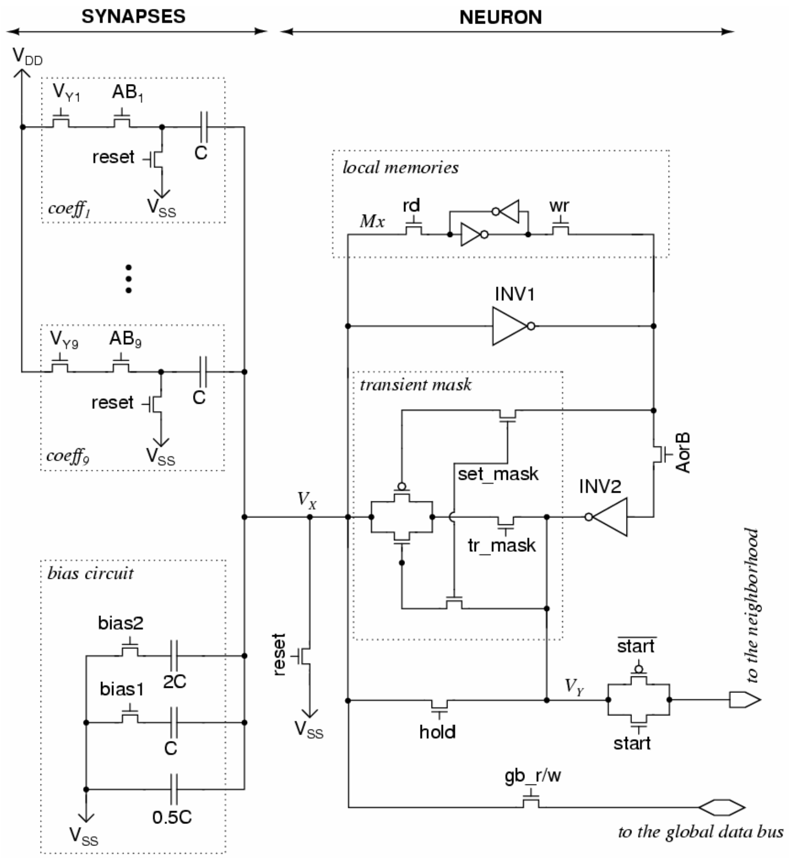

Figure 2.4.5. Binary-programmable CNN cell based on the floating gate MOS structure.

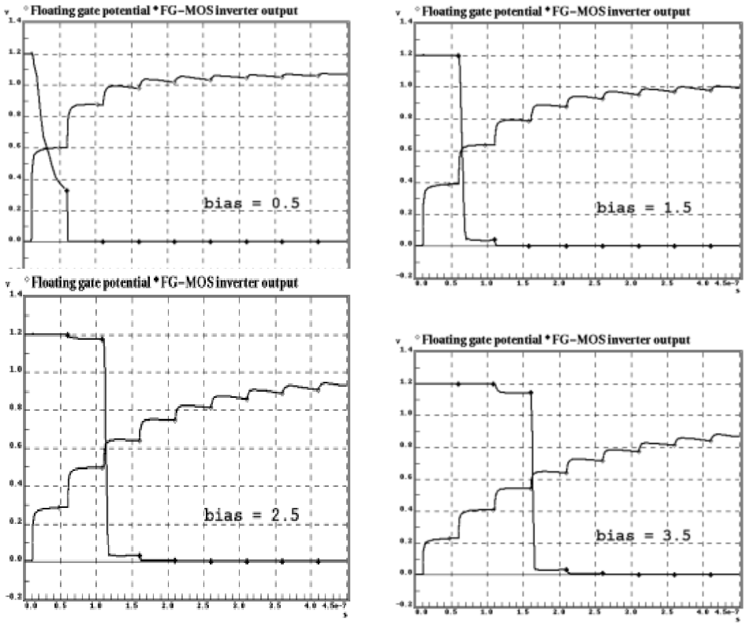

Figure 2.4.6. Simulated neuron activation at threshold (bias) programmed to 0.5, 1.5, 2.5, and 3.5.

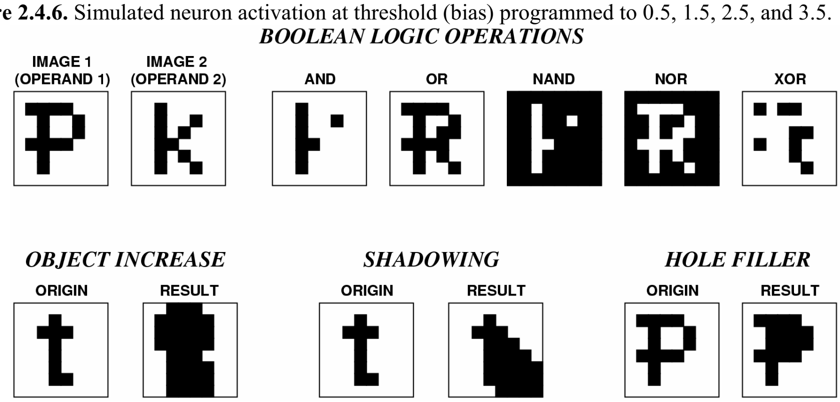

Figure 2.4.7. Network simulation results: Boolean logic functions, *Object Increase* operation, *Shadowing*, and *Hole Filler* operation. Black pixels correspond to logical high value.

Single electronics is an appealing concept for ultra-low power electronic systems that encode the information with a countable amount of electrons. When the technological progress of fabrication facilities enabled the production of devices with feature sizes in nanometer scale the idea of single electronics becomes even more attractive. Among the promising nanotechnology concepts, the single-electron tunneling (SET) technology occupies a prominent place. It is based on relatively well-investigated phenomena like Coulomb interactions, quantum confinement and tunneling. A basic element in this technology is a tunnel junction. It consists of two conductors (or semiconductors) separated by a very thin insulating layer sketched in Fig.2.4.8. Such a junction is equivalent to capacitor as long as no tunneling event takes place. However, the insulation layer is so thin that electrons can tunnel through the potential barrier if certain conditions are met. Figure 2.4.9. presents energy levels in the junction. When no external excitation is applied, the energy Fermi levels, $\boldsymbol{E_{F1}}$ and $\boldsymbol{E_{F2}}$, are in-line (equal). In this case no electron tunneling is possible – the junction is in the state called "Coulomb blockade". However, if additional energy is supplied, e.g. the junction is connected to a voltage source the energy levels will be shifted by

$$\Delta E = E_{F1} - E_{F2} = e \cdot V \tag{2.43}$$

where: $\boldsymbol{\Delta E}$ is the energy shift resulting from the applied voltage $\boldsymbol{V}$, and $\boldsymbol{e}$ represents an electron charge. The tunneling event occurs if the supplied energy ΔE exceeds the Coulomb energy $E_C = e^2/(2C)$.

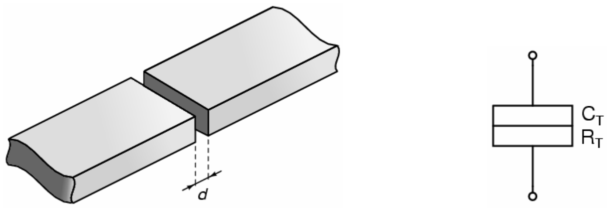

Figure 2.4.8. Structure and the symbol representation of a SET junction.

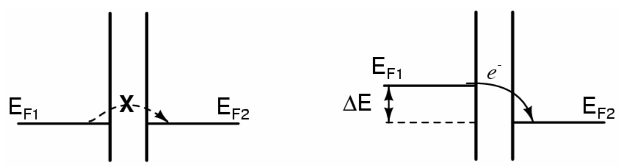

Figure 2.4.9. Potential barriers in SET junction without and with external excitation.

There are two main parameters characterizing the junction:

- tunnel capacitance, $C_T \propto 1/d$, defined by the size of the junction and materials used for its fabrication;
- tunnel resistance, $R_T \propto d^2$, which is dynamic parameter defined as the voltage across the junction divided by the current flowing through the junction.

The simplest structure built with SET junctions is a SET transistor. It consists of two tunnel junctions connected in series via a very small conducting island (quantum dot). Drain-source bias is applied across the junctions while the island is capacitively coupled to gate inputs. The model of a SET transistor is shown in Fig.2.4.10. If the substrate under the device is connected to either supply voltage or ground potential, the stray capacitance functions as a bias gate. In this way, the N- and P-type devices are obtained, and CMOS-like complementary circuits can be built. A very interesting feature of a SET transistor can be observed in its current-voltage (I-V) characteristics shown in Fig.11., where the drain current and the island charge are plotted versus the gate voltage. When the input gate voltage spans a range many times wider than the drain-source bias voltage, periodic current peaks appear due to the electrons transferred to and from the island. This phenomenon is called Coulomb oscillations.

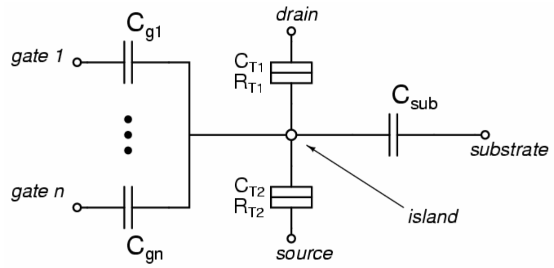

Figure 2.4.10. Model of a SET transistor.

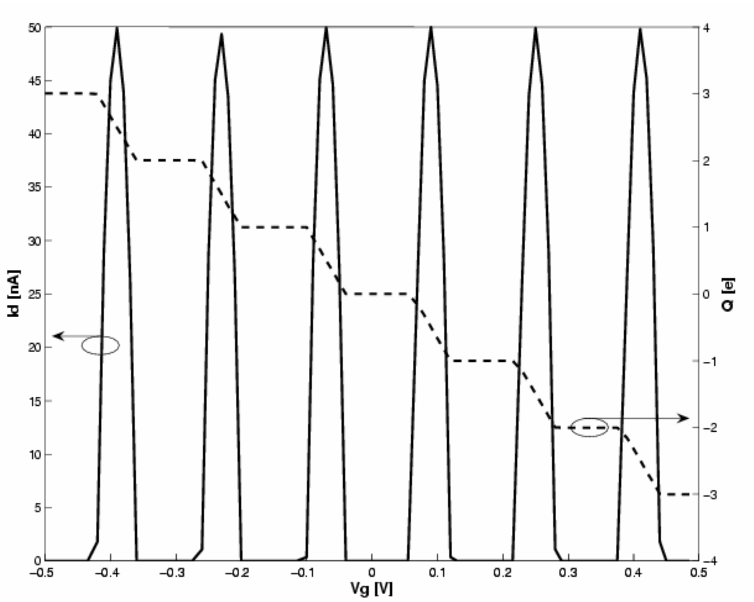

Figure 2.4.11. The drain current of a SET transistor and the charge of the island (expressed in number of electrons) as a function of the gate voltage. Simulation parameters: $\boldsymbol{T}$ = 0K, $\boldsymbol{C_T}$ = 1aF, $\boldsymbol{R_T}$ = 100kΩ, $\boldsymbol{C_g}$ = 1aF, and $\boldsymbol{V_{DD}}$ = 10mV.

Based on the experience gained during the development of FG-MOS CNN, a SET implementation of a processing cell, shown in Fig.2.4.12., has been proposed. The designed circuit follows the McCulloch and Pitts neuron model. SET inverter forms the backbone of this circuit, which is quite standard approach [RH2004]-[GG2004]. The novelty of this design lies in the synapse circuitry, which is a direct derivative of the structure developed for the FG-MOS CNN. In addition, the threshold implementation and programming scheme are analogous. The neighborhood outputs, $\boldsymbol{V_{Yi}}$, control the P-type SET switches, and thus a second inverter in the neuron structure is not needed. Since the template terms, $\boldsymbol{AB_i}$, are global signals, the corresponding switches can be implemented with either MOS or SET devices. Therefore, the proposed structure is suitable for both pure SET and SET-FET hybrid implementations. Additionally, the unit capacitances are much easier to implement than weighted as in Reference [GG2004], due to the accuracy requirements. The coupling capacitance of 80aF and 1aF tunnel junctions can be fabricated with desired matching accuracy. However, for the room temperature operation a further downscaling is needed.

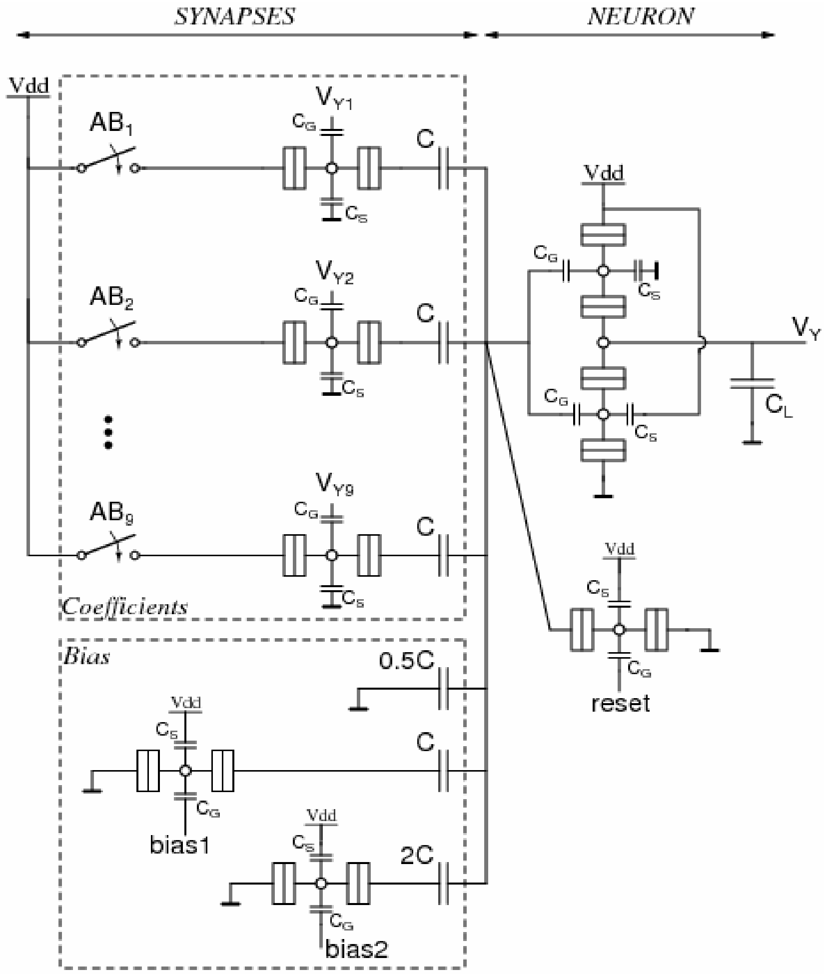

Figure 2.4.12. CNN cell structure designed for implementation with SET technology.

The designed circuit has been simulated with the following set of parameters $\boldsymbol{C_T}$ = 1aF, $\boldsymbol{R_T}$ = 100kΩ, $\boldsymbol{C_g}$ = 6aF, $\boldsymbol{C_{sub}}$ = 4.5aF, $\boldsymbol{C}$ = 80aF, $\boldsymbol{C_L}$ = 35aF, $\boldsymbol{V_{DD}}$ = 10mV, and $\boldsymbol{T}$ = 400mK. The computation by means of charge distribution is shown in Fig.13., and the dynamic power consumed by the inverter is visualized in Fig.14.

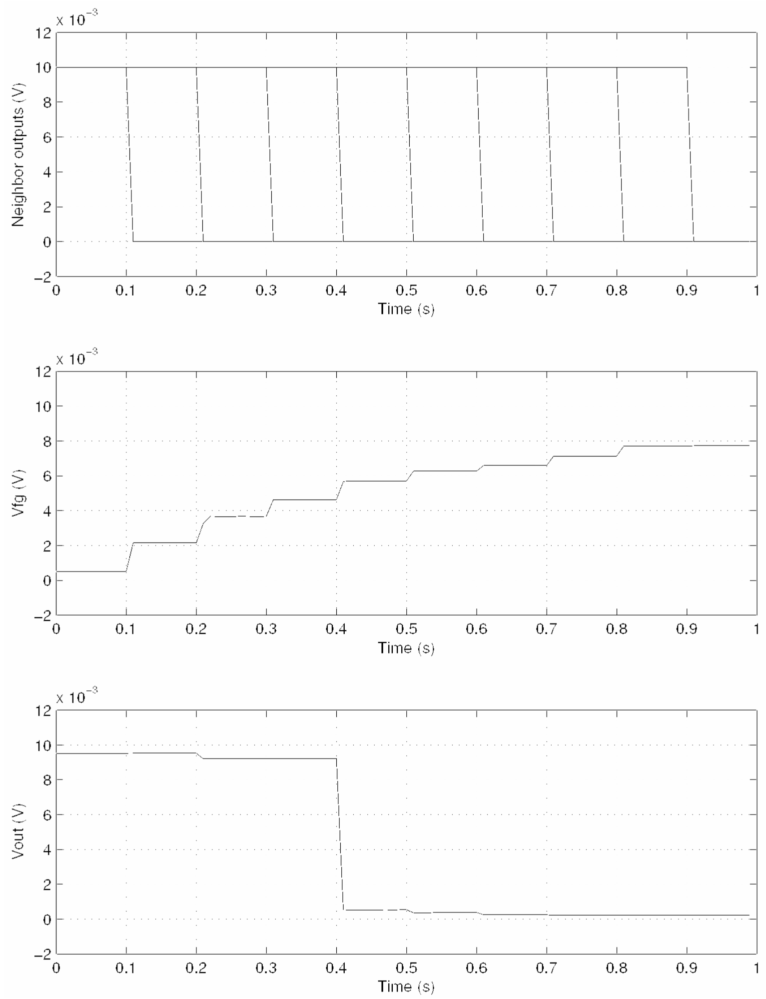

Figure 2.4.13. Cell operating principle. Neighborhood outputs activate the synapses causing the floating node potential to rise. For the number of active synapses larger than bias (set to 3.5 in the shown case), the floating node potential exceeds the comparator threshold of $V_{DD}/2$ and the neuron output triggers.

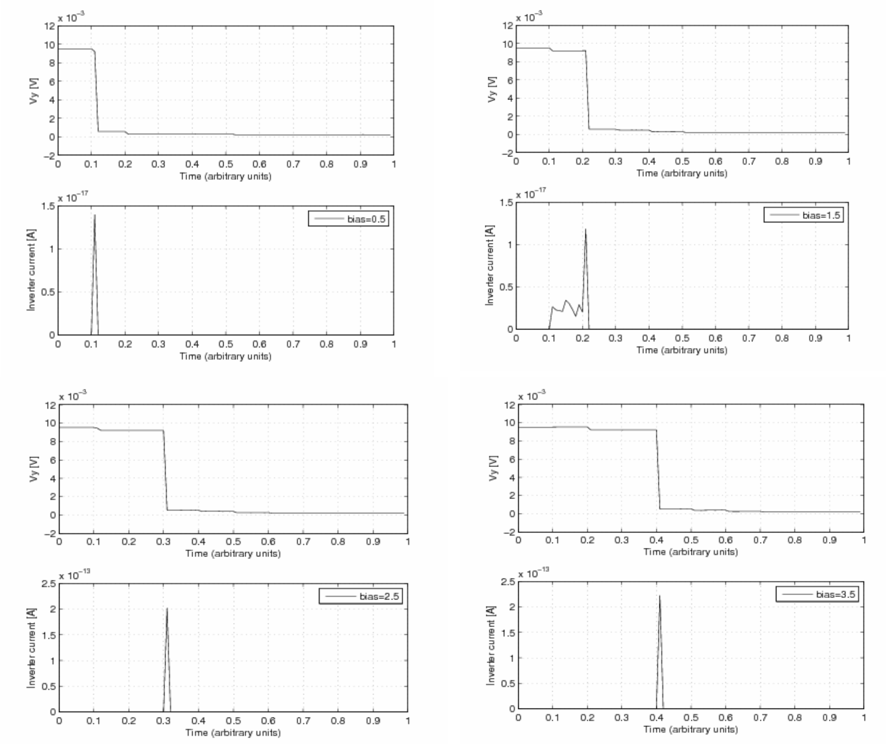

Figure 2.4.14. The output voltage and the current dragged from the supply source by the inverter at different bias values.

To build a powerful array processor, a large network of processing elements is required. Attempts to implement it efficiently on chip bring a number of issues to face. The small layout-area and the low power-consumption are critical. From this point of view, an implementation with SET devices becomes very attractive. The cell structure is kept small and bears the possibility for further downscaling. The power dissipation is kept low as well. With coupling capacitors of 80aF, the floating node can store up to about 60 electrons. In addition to the energy-efficient voltage-mode summation, the complementary structure of the inverter minimizes the static power consumption. Moreover, the extremely low supply voltage of only 10mV keeps the dynamic power consumption low. According to simulations, the current dragged by the inverter during the switching is in the range of 10^{-13}A. These results show how extremely low supply power is sufficient for operation of SET circuits. A more detailed description and discussion of this design can be found in References [C8] and [D4].

The presented design is probably the first programmable CNN implementation in SET technology. The adopted binary-programming scheme is fast and robust, and certainly makes the cell one of the most versatile nanoimplementation of CNN. Most of the templates handling B/W images can be computed with the presented structure. However, to take a full advantage of the applied programming scheme, the cell structure needs to be extended. Namely, the transient mask is needed for computing local logic functions as well as for fixed state map implementation. Additionally, local memories are required for the algorithmic evaluation of more complex operations. After providing the cell with these extensions, evaluation of all B/W operations would be possible.

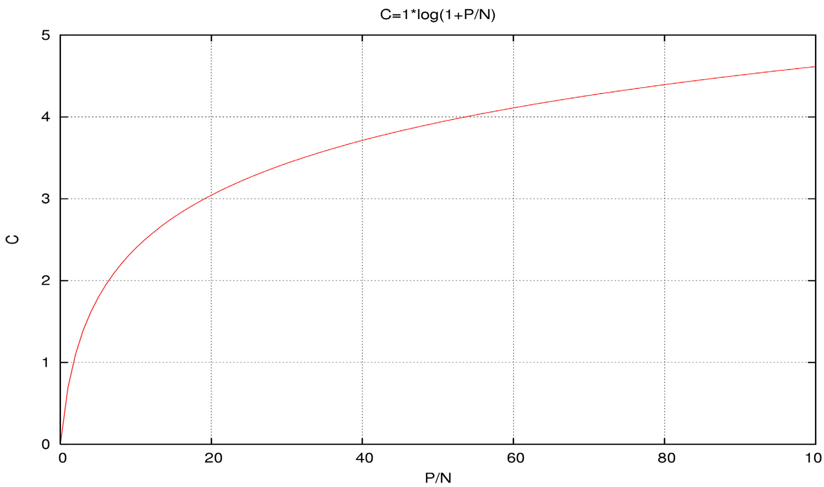

Figure 2.5.1. Channel capacity normalized to band width.

2.5 Integrated System Circuits, VTT

Subproject objectives

The set objectives of this subproject were to study biological information processing and apply the principles learned on electrical engineering to construct bio-inspired circuit blocks. The emphasis in the design work was to be on the same features that are found in the nature's information processing systems: parallelism, robustness and low-energy operation.

Motivation for bio-inspired information processing

The brain and the nervous system are very energy efficient in their information processing. Comparison between conventional CMOS technology and the human brain shows that man made systems use many decades more energy per operation that the biological counterpart does. It can approximated that the amount of energy per elementary operation in the brain is order of 3.3 fJ [Mea90] and in a 0.35 µm CMOS transistor 55 fJ, [MÅ04] respectively. Furthermore, the elementary energy per operation for a complete system is much higher than switching power of a transistor is.[Mea90]
Biological information processing systems are evolved to be suitable for theirs tasks. The absolute performance and energy consumption are in harmony, and the systems adapt to the environment. [eee00] Thus the biological systems make a very attracting model for low-power electronic devices.

Energy efficiency

Shannon-Hartley's theory predicts that channel capacity C in bits is related to it's bandwidth W and signal-to-noise ratio S in the following way:

$$C = W \log(1+S) \qquad \text{(eq. 2.5.1)}$$

From figure 2.5.1 it can be seen, that the signal-to-noise ratio requirement grows faster than channel capacity.

Digital information processing is a simple way to achieve high precision but it uses a lot of resources, that is area on silicon and energy. [Sar98]
In analog signal processing, noise accumulates stage after stage according to Friis' formula:

$$F = F_1 + \frac{F_2 - 1}{G_1} + \frac{F_3 - 1}{G_1 G_2} + \ldots + \frac{F_n - 1}{G_1 G_2 \cdots G_{n-1}} \qquad \text{(eq. 2.5.2)}$$

On the other hand, analog signal processing is economic at low precision. Furthermore, physical properties of analog components can be used as primitive computational functions. [Sar98] The precision limit is technology dependent, approximations vary between 4-5 bits [FP96] and 8-10 bits. [Sar98] So below that limit analog computing is more energy efficient and for higher precisions digital, respectively.
Biological information processing systems have both digital and analog computational characteristic. [Sar98] Neurons receive pulses, or spikes, from other neurons and integrate the received signals. [Lis97] On the other hand, neurons also use graded potentials for communication. [dRvSL96]
The part of organism's energy budget the brain and the nervous systems use can be substantial. Signal processing in biological systems uses many parallel low-power channels and is distributed to save energy. [LdRvSA98, Lau01] It's apparently restrained energy availability that has led the evolution to the direction which favors energy efficient systems which code information efficiently. [LB96, Sar98]

Property	***Analog***	***Digital***	***Hybrid***
Precision	High expensive	Very high possible	High at system level
Noise	thermic, 1/f	Rounding errors	rounding, physical
Noise accumulation	Every stage	Signal level restoration	Partly level restoration
Bits/channel	Many	One	Some
Computational primitives	Physical properties	Logical operations	Physical and/or logical
Number of wires	Low	High	High to medium
Voltage levels	~mV	>1 V	~200 mV (biological)
Energy efficiency	Low S/N: good	High S/N: good	Optimum for a task

Table 2.5.1: Comparison between analog, digital and hybrid mode signal processing. [MÅ04]

Neuromorphism

One can take different kind of viewpoints when drawing ideas from biological information processing systems to build better than ever electronic devices. One is to know the very construction of the biological system and replicate it on silicon. The other is to take concepts and ideas, and then to apply then on the available technology. Although the latter is probably more fruitful from the point of IC designers view, the following principles are proposed to be followed in both cases: [M4]

1. Observe and study functioning of the brain and nervous system
2. Analyze the observations and verify the results quantitatively with information theory
3. Apply the result on existing circuits, but also design all new circuit blocks. New algorithms are needed to fully exploit the possibilities.

The application of aforementioned features of biological information processing can be summed up in the following way: [M4]
Distribution and parallelism: Signal preprocessing to save communication and processing costs. Use many parallel optimum precision channels for energy efficiency.
Hybrid mode operation: Pulse mode is used when robustness is needed over a long communication channel. When high information rate near distance communication is required, analog mode is probably more efficient.
Computational primitives: Exploit physical features of a component to carry out computation.
Coding: Suitable signal coding can significantly improve robustness and can be used in nonlinear calculations. Coding enabling highest possible information rate is not necessarily the most energy efficient one.

Experimental ADA block

ADA block is a building element which implements basic signal restoration scheme for hybrid mode computation. When signal is distorted in analog stages by noise and component unidealities, ADA restores signal to well defined levels. The block fundamentally implements successive AD and DA conversion. Figure 2.1.2 shows ADA output characteristics and figure 2.5.3 a possible block diagram of a systems utilizing ADA blocks. [Sar98]

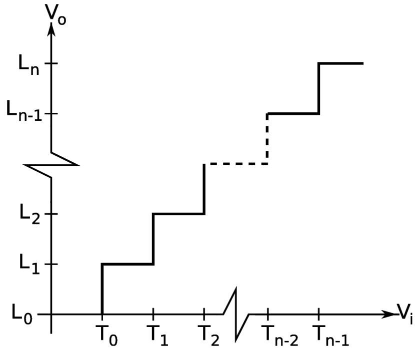

Figure 2.5.2. ADA input versus output graph.

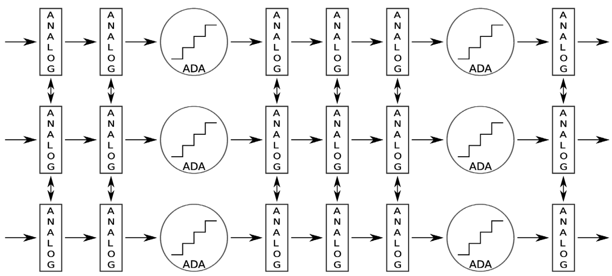

Figure 2.5.3. Analog parallel system utilizing ADA block.

In order to validate the idea of hybrid computation and test the observations of biological systems' features, a system consisting of ADA blocks were designed, analyzed, simulated and implemented. [M4]

The designed experimental system consists of five ADA blocks. The design allows it be used to test system's robustness to component malfunction, noise immunity, parallelism and hybrid mode computation.

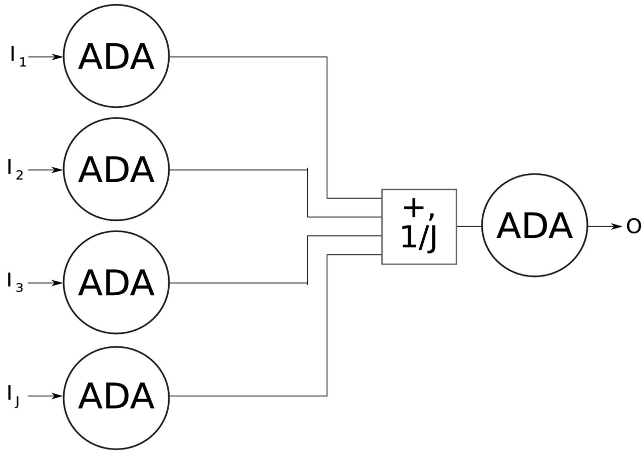

Figure 2.5.4. Experimental system of ADA blocks.

A probability theoretic analysis of systems ideal case noise immunity were carried out, which shows that parallelism can be used to make more noise immune systems. The result can also be interpreted so that it is possible to use poor components in parallel and still build functional systems, and using components of low quality can be very beneficial in regard to energy efficiency and area expenditure on silicon.

Conventional CMOS process was chosen for implementation. The single ADA design makes use of floating gate (FG) transistors. As explained in section 2.3, FG-MOS is well suited for low-power applications. FG-MOS technique is also neuromorphic in it's very nature: biological neuron signal integration is mimicked by capacitive summing and makes most of the physical properties of the structure.

The operating point of the core of the ADA block were designed to be in deep sub threshold operating area. Sub threshold operation of a transistor is quite different from saturation area operation. The physical transfer phenomenon of the sub threshold operation is charge carrier diffusion, when in strong inversion the channel current is mainly due to drifting.

subvth kaavat. (eq. 2.1.3)

Although sub threshold operation is thoroughly known, it's not a very widely used technique. As can be seen from the equation 2.1.3, sub threshold current is exponentially dependent on the control voltage and V_M, which make it susceptible to manufacturing variations. Sub threshold current is also very small compared to strong inversion current, which makes the operation slow. [Tsi99] Thus sub threshold technique is usually in use in special applications only, such as peacemakers and swatches which require ultra-low energy consumption.

Although the reasons above inhibit using sub threshold technique in conventional circuits, it can be used in neuromorphic circuits: neuromorphism helps to overcome the downsides of technique and benefit from the good features, namely ultra-low energy consumption.

Figure 2.1.5 shows core block of the ADA (marked *a* in figure 2.1.6). Both NMOS and PMOS transistors operate in sub threshold domain. All the NMOS transistors share

common inputs for signal V_i and bias V_{bn}, which are summed on the floating gate. Respectively, all the PMOS transistors share common bias V_{bn}. The output of the block is essentially output of an array of four inverters with evenly distributed trip points. Basically, the block implements the AD part of the ADA.
DA part of the block is done in a simple capacitive summing block (marked c in figure 2.5.6). Picture 2.5.6 shows the block diagram of ADA component.

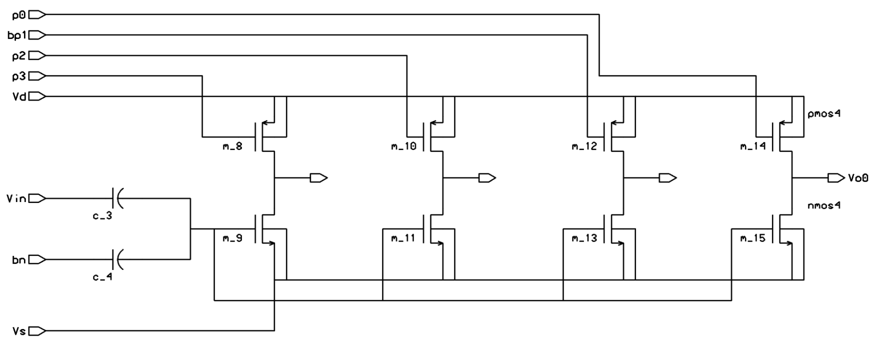

Figure 2.5.5. Block which carries out AD conversion.

The analysis results and the designed system were compared. Simulations show, that the system of ADA blocks shows noise immunity and resistance to component failures over a single ADA. Figures 2.5.9 shows systems output when one systems input is stuck at ground potential. As can be seen, the performance degrades, but does not collapse. From figures 2.5.7 and 2.5.8 what happens when evenly distributed noise is added to the input signal. As can be seen, the system has improved noise tolerance, which is due to parallelism, over a single ADA block.Simulated typical power consumption for one core block in figure 2.5.5 was approximately between 0.1 nW and 1 nW depending on the input signal. ADA block's power consumption is considerably higher. This is due to the fact that the block was design of an ADA block was intended to be on the safe side what comes to building the system of ADAs.

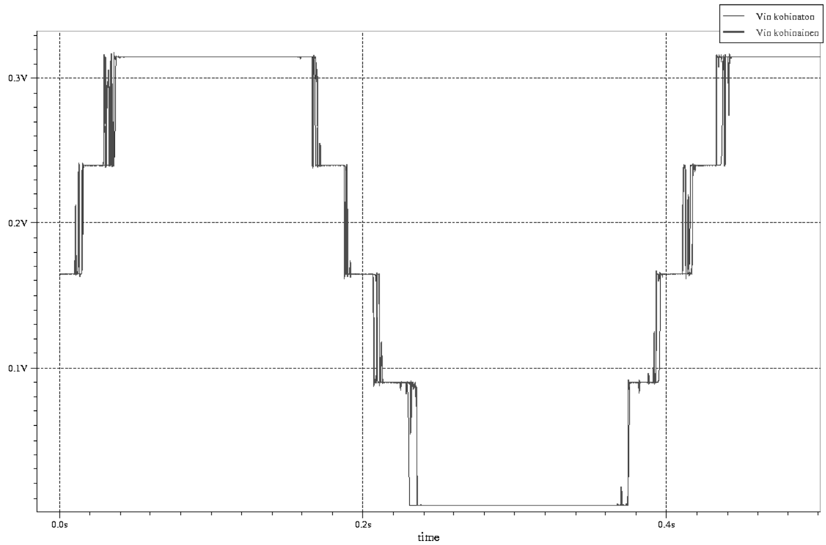

Figure 2.5.7. Output of an ADA block with ideal input (blue) and with noisy input (red).

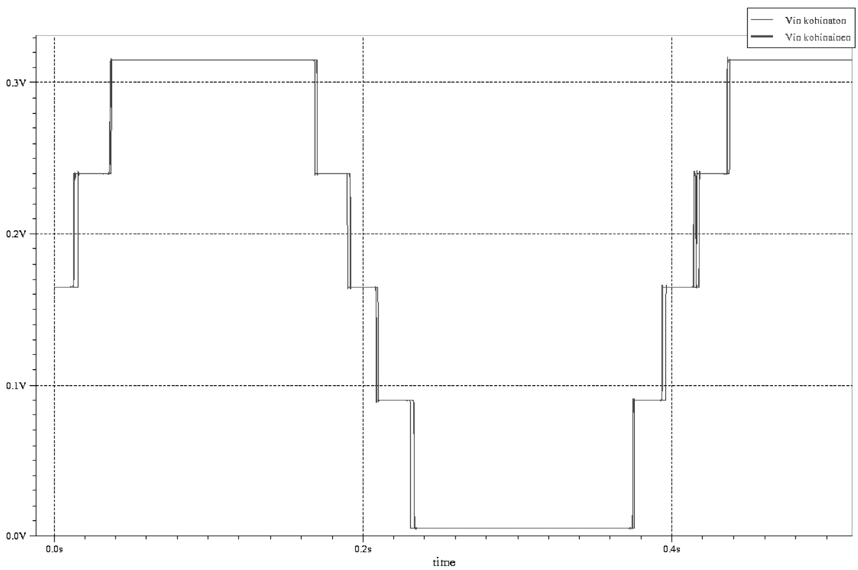

Figure 2.5.8: Output of the ADA system with ideal input (blue) and with noisy input (red).

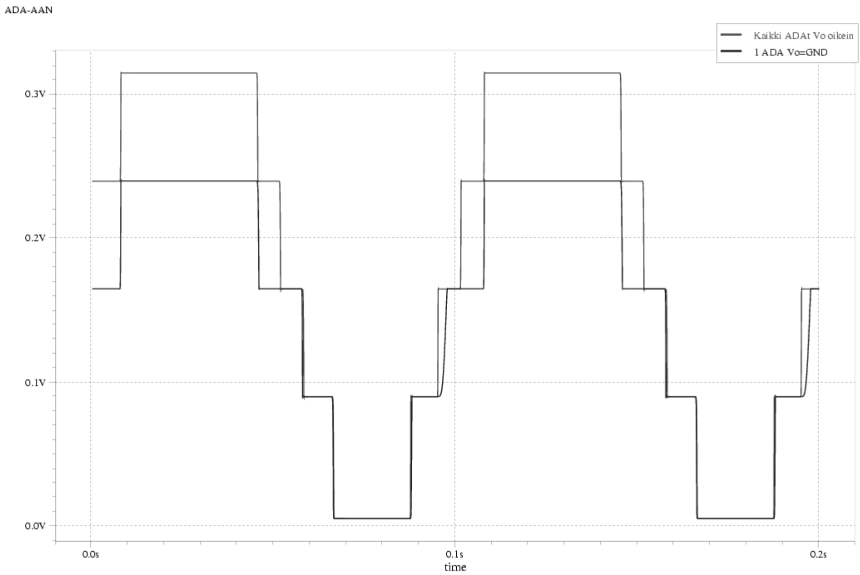

Figure 2.5.9. ADA system with one input stuck at ground potential (blue) and all inputs correct (red).

Measurements

Measurements were designed to verify sub threshold operation of ADA's building blocks, bias trimming operation and the system's supposed benefits over a single ADA block.
Two chips were processed. Initial measurements of the showed that there is an threshold voltage offset of several voltages on gates of FG-MOS transistors. The result was that the ADA block showed nonzero output only after several voltages were applied on the input. This strongly conflicts with the calculations, simulations and process parameters. After further measurements, discussions with the manufacturer and literature study [KF96, RVB03, RVYRY03] it was concluded that there is trapped charge in the floating gate which shifts the effective threshold voltage on the gates.
Charge trapped on floating gate during manufacturing can be removed with a special passive structure. [RBV03] The structure is a simple contact stack which connects floating gate to the top metal layer. Since there is a temporal galvanic connection from floating gate to every metal layer during manufacturing, the charge accumulated can freely flow away from the gate. After top layer metal it etched there is no connection from floating gate anymore.
The blocks were altered according to this scheme and second ship was processed. Also blocks without the contact stack were placed on the chip for comparison purposes.
Unfortunately, the measurements showed forthwith that the contact stack has not worked. The blocks with or without the stack showed similar threshold offset. The offset was also comparable to to offset on the blocks of the first chip.
Extensive measurements were carried out to verify the reason of the offset. As figure 2.5.10 shows, it was possible to connect the NMOS transistors utilizing floating gate (block *a* in figure 2.5.6) so that it was possible to measure properties of single transistors. The measurements and calculations confirmed that the transistors were manufactured successfully. The same was true for PMOS transistors in the block.

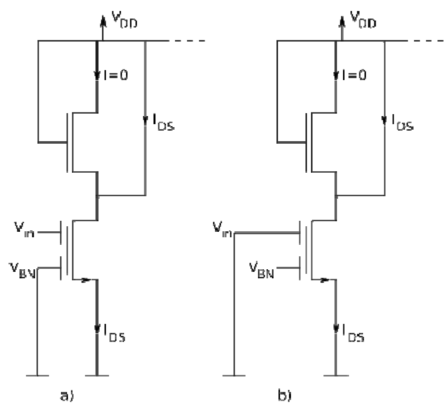

Figure 2.5.10. Setup for verifying FG-NMOS operation.

Is was not possible to break insulation between floating poly silicon and input with over voltage to free the trapped mobile charge without breaking gate oxide. Luckily, one input of one block of a specimen were broken supposedly due to static discharge. With connecting the inputs as in figure 2.5.10 a) it was possible to measure a normal transfer graph of a NMOS transistor as well as verify that the threshold voltage is as expected.
All summarized, there is strong evidence that the offset is caused by mobile trapped charge. FG structures of the same kind has been used with success with the same process before. [RFK+01, RSÅ04] It remains unknown why it was that the charge removing stack structure did not work and why specifically this circuit was plagued by floating gate trapped charge.
Despite that trapped charge prevented testing the system of ADA blocks, it was possible to verify that the ADA block's design principles are plausible.

SET structures

VTT Microelectronics has fabricated SET structures with different number of gate electrodes on SOI substrate. The thickness of the SOI film was first reduced to 40 nm by thermal oxidation. The SETs were defined by electron beam lithography and dry plasma etching. After etching the width of the conducting channels was further reduced, and thus charging energy enhanced, by an additional thermal oxidation step. Figure 2.5.11 (a) presents a scanning electron micrograph of an SET with four separate gate electrodes. So far a set of samples with one or two gates has been characterized at 4.2 K. Figure 2.5.11 (b) illustrates a typical strongly non-linear source-drain *IV*-characteristic with high dynamical resistance close to zero bias, which is a manifestation of a Coulomb charging effect. The gate voltage modulation of the source-drain current I_{DS} was also measured by applying a small constant source-drain voltage and by measuring current against the voltage(s) in the gate electrode(s). Figure 2.5.12 presents a typical result measured from a two gate device. It shows that I_{DS} exhibits clear Coulomb oscillations in both gate voltage directions, and the phase of the oscillations can be tuned by the other gate voltage. The performed measurements clearly demonstrate that the working point of the device can be tuned with an additional gate control and that multiple gate SETs can be used for performing logical operations.

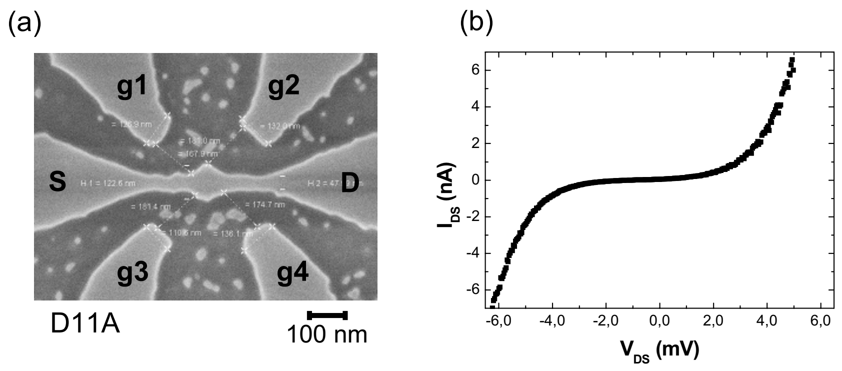

Figure 2.5.11. (a) Scanning electron micrograph of an SET with four gate electrodes. (b) Typical strongly non-linear *IV*-characteristic measured at 4.2 K.

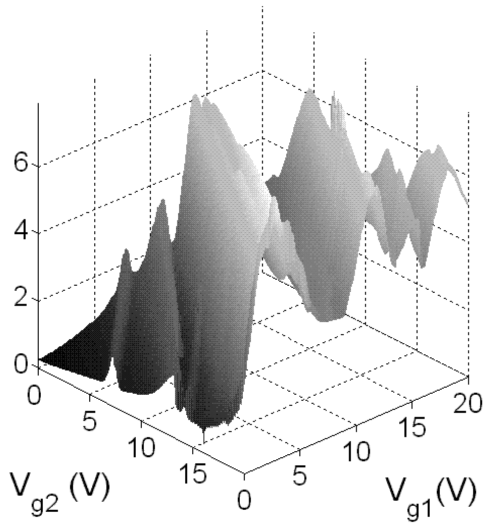

Figure 2.5.12. Map of source-drain current I_{DS} measured at 4.2 K from a two gate device as a function of the two gate voltages. The constant source-drain bias voltage bias was approximately 3 mV.

2.6 University of Oulu, Biophysics

The biophysics subproject has been concentrating on the stochastic nature of the graded (strictly analog) signalling between neurons, and the energy consumption therein. In the course of the past years (2003-2004) we have formed some preliminary models on the basis of experimental work, especially concerning the non-linear ("voltage-dependent") nature of the cell membranes and of the synaptic signal transfer. The models reproduce some properties of cellular communication, but the models still do not include reasonable estimates of energy consumption.

However, during 2004-6 the large, modular compound eye of the American cockroach was studied as a research model. This lead to a hypothesis, according to which one of the main factors of seeing well in low luminance was combination of random sensor functions of individual photoreceptors, high non-linearity and large spatial summation of signals [13] (Heimonen et al, 2006). This hypothesis, and the preliminary computer modelling of the processes points to possibilities of implementing similar signal processing systems in artificial circuits.

3 Annual meetings of the consortium and international aspects

In addition to the bilateral contacts and collaboration the consortium has had three annual meetings October 10 2003, January 13 2004 and April 25 2005 during which the research plan and progress reports has been discussed.

LCE has been collaborating with the Institute of industrial science of the University of Tokyo (prof H. Sakaki) on compound semiconductor and SOI materials.The biophysics group has been collaborating with a group in Univ. of Bielefeld (prof. Martin Egelhaaf, Dept. of Neurobiology) and a group in Univ. of Cambridge (prof. Simon Laughlin and Dr. Jeremy Niven, Dept. of Zoology), on the topic of graded potential signalling in the nervous system.

4 Publications and Academic Degrees

Table 2. Publications and academic degrees produced in the project. Numbers of different types of publications are given along with the reference numbers. List of refereed journal articles are given in Section 5.1, refereed conference papers in Section 5.2, monographs in Section 5.3 and theses in Section 5.4.

Partner	Type of publication	2003	2004	2005	2006	**Total**	Publication numbers
LCE	Ref journal artic.	-	1	0	4	**5**	1-5
	Ref. conf. papers	-	-	-	1	**1**	C10
ECDL	Ref. journal art.	-	-	-	2	**2**	15-16
	Ref. conf. papers	-	3	3	2	**8**	C1-8
VTT	Ref. conf. papers	-	1	-	1	**2**	C9-10
	Master degrees	-	-	-	1	**1**	
OY	Ref. journal art.	2	2	2	3	**9**	6-14
	Ref. conf. papers	3	-	-	-	**3**	C11-13
All labs	Doctoral dissert.	1	-	-	1	**2**	2 scheduled 2007
"	Master degrees	1	-	-	3	**4**	

5 Publications

5.1 Refereed Journal Articles and book chapters

[1] F. Boxberg and J. Tulkki, *Quantum Dots: Phenomenology, Modeling and simulations, Photonic properties and Applications***,** in Handbook of Nanotechnology: Nanometer Structure Theory, Modeling and Simulation Edit**.** A. Lakhtakia, SPIE (2004).

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[3] J. Oksanen and J. Tulkki, *Fast coherent all-optical flip-flop memory*, Appl. Phys. Lett. **88**, 181118 (2006).

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[10] M. Vähäsöyrinki, J. E. Niven, R. C. Hardie, M. Weckström & M. Juusola. *Robustness of contrast coding in Drosophila photoreceptors in the absence of slow delayed rectifier K+ channels* (submitted to Nature Neurosci.)

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[16] M. Laiho, A. Paasio, J. Flak, and K. Halonen, Template Design for Cellular Nonlinear Networks with One-Bit Weights, accepted to the IEEE Transactions on Circuits and Systems, 2006.

5.2 Refereed Conference Papers

[C1] A. Paasio, J. Flak, M. Laiho, K. Halonen *High Density VLSI Implementation of a Bipolar CNN with Reduced Programmability*. Proceedings of IEEE International Symposium on Circuits and Systems ISCAS 2004, Vancouver, Canada, pp. III-21 – III-24. (2004).

[C2] J. Flak, M. Laiho, A. Paasio, K. Halonen *VLSI Implementation of a Binary CNN: First Measurement Results*. Proceedings of The 8th IEEE International Workshop on Cellular Neural Networks and their Applications CNNA 2004, Budapest, Hungary, pp. 129 – 134. (2004).

[C3] J. Flak, M. Laiho, A. Paasio, K. Halonen *Cell Structure for a Capacitively Coupled Binary CNN.* Proceedings of Biannual Baltic Electronics Conference BEC’04, Tallinn, Estonia, pp. 103 – 104. (2004).

[C4] J. Flak, M. Laiho, K. Halonen *FG-MOS Neuron for Binary CNN*. Presented at the SPIE symposium “Microtechnologies for the New Millennium 2005”, Seville, Spain. To be published in the Proceedings of SPIE, vol. 5839, paper no. 5839-37. (2005).

[C5] M. Laiho, J. Flak, A. Paasio, K. Halonen *Template Design for a Binary-Programmable Cellular Nonlinear Networks*. To be presented at the 2005 IEEE International Symposium on Circuits and Systems, Kobe, Japan, 23-26 May 2005. (2005).

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[C7] J. Flak, M. Laiho, and K. Halonen, On Emerging Nanodevices and Architectures, Proceedings of the 10th Biennial Baltic Electronics Conference (BEC 2006), Tallinn, Estonia, pp. 67 – 70, 2006.

[C8] J. Flak, M. Laiho, and K. Halonen, Programmable CNN Cell Based on SET Transistors, Proceedings of the 10th IEEE International Workshop on Cellular Neural Networks and their Applications (CNNA 2006), Istanbul, Turkey, pp. 182 – 185, 2006.

[C9] J. Mäkipää and M. Åberg, *Energy Efficiency Through Neuromorphism*, Baltic Electronics Conference, Tallin, Estonia, October 3-6, 2004, (2004)

[C10] Jani Mäkipää and Teppo Häyrynen, "Hybrid analog-digital multilevel signal restoration: comparison between CMOS and SET technologies", in Nanotechnology in Northern Europe conference, 2006.

[C11]Weckström M, Heimonen K, Kauranen M & Vähäsöyrinki M . *Role of the microvillar membrane in electrical properties of insect photoreceptors.* Göttingen Neurobiology Conference 2003, Thieme Verlag. (2003).

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[C13]Vähäsöyrinki M, Weckström M, Juusola M & Niven J *Information processing during light adaptation in blowfly photoreceptors*. Göttingen Neurobiology Conference 2003, Thieme Verlag.(2003).

5.3 Doctoral, Licentiate, and Master Theses

<u>PhDs</u>

[D1] Mikko Vähäsöyrinki: *Voltage-gated K+ channels in Drosophila photoreceptors.* Acta Univ Oul A426, (2003).

[D2] J. Oksanen: Modeling transmitters, amplifiers and nonlinear circuits for the next generation optical networks, HUT thesis (2006).

[D3] J Saijets, PhD thesis in preparation on advanced CMOS modelling, under pre-examination, defense (2007).

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[M5] T. Häyrynen, *Quantum transport in the ballistic and Coulomb blockade regimes*, Masters thesis, (2003).

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NANOSENSORS (NASE)

Project leader: Prof. Päivi Törmä (P1) [1]
Subproject leaders
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Academy Fellow Sorin Paraoanu (P2.2)[3]
Prof. Jorma Virtanen (P3)[4]
Prof. Matti Vuento (P4)[5]
Prof. Kari Rissanen (P5)[6]
Prof. Matti Manninen (P6)[7]
Prof. Markku Kulomaa (P7)[8]
Prof. Jouko Korppi-Tommola (P8)[9]

Abstract

In this project we focus on nanosensors, more specifically on 1. Nanosensors for temperature, 2. Nanosensors utilizing DNA and carbon nanotubes. University of Jyväskylä has long term experience on thermal effects in nano- and microstructures, which has lead for instance to spin-off companies. We bring the research on nanothermometry to new areas such as thermometers for individual living cells. The development of this kind of applications is supported by basic research on thermal effects in nanostructures. Carbon nanotubes and DNA-molecules are probably the most promising candidates for organic nanoelectronics, and DNA is interesting on its own due to its connection to life. The research on these topics relies on close collaboration between experts in electronics, physics, chemistry and biology.

The research effort is divided into three work packages (WP). WP1 "Bio-nanonelectronics" considers two specific topics: trapping of macromolecules and DNA conductivity, as well as cell thermometry. WP2 considers molecular electronics based on carbon nanotube rotaxanes. Especially, optical properties are considered. WP3 "Thermal effects in nanostructures" concentrates on experimental and theoretical basic research on electron transport and thermal effects in nanosctructures.

1 Partners and Funding

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1.1 Nanoelectronics group, Prof. P. Törmä, Nanoscience Center, Department of Physics, University of Jyväskylä (P1)

The research group at the moment consists of subproject leader Prof. Päivi Törmä, senior researcher Dr. Jussi Toppari, postdoc Dr. Andreas Johansson, Ph.D. students Sampo Tuukkanen (Ph.D. achieved in the end of 2006), Tommi Hakala, Anton Kuzyk, Marcus Rinkiö, and M.Sc. students Marina Zavodchikova and Veikko Linko. Earlier M.Sc. students who worked on this project were Mikko Laitinen, Lasse Hirviniemi and Heli Lehtivuori.

1.2 Experimental nanophysics group, Academy Fellow I. Maasilta, Nanoscience Center, Department of Physics, University of Jyväskylä (P2.1)

The research group currently consists of subproject leader Academy research fellow Maasilta, postgraduate students Jenni Karvonen, Kimmo Kinnunen, Panu Koppinen, Minna Nevala and and Master's students Tero Isotalo and Henri Jaakkola.

1.3 Nanophysics/Quantum Engineering group, Academy Fellow S. Paraoanu, Nanoscience Center, Department of Physics, University of Jyväskylä (P2.2)

The research group consists of subproject leader Dr. Gheorghe-Sorin Paraoanu, graduate students V. Haaksluoto and S. Ylinen, and postgraduate students J. Lie and K. Chalapat. Earlier, also graduate students A. M. Halvari and M. A. Hassan have worked on this project. On the theoretical part of the project, the research group has also included postgraduate student T. Kuehn (from Prof. M. Manninen group).

1.4 Group of Prof. J. Virtanen, Nanoscience Center, Department of Chemistry, University of Jyväskylä (P3)

The research group consists of subproject leader Prof. Jorma Virtanen and Ph.D. student Suvi Virtanen.

1.5 Group of Prof. M. Vuento, Nanoscience Center, Department of Biological and Environmental Science, University of Jyväskylä (P4)

M. Vuento (subproject leader), Jonna Nykky, (Ph.D. student), Hanna Lindholm and Hanna-Leena Putkinen (M.Sc. students).

1.6 Organic Chemistry Laboratory, Nanoscience Center, Department of Chemistry, Prof. K. Rissanen, University of Jyväskylä (P5)

The research group for this project consists of subproject leader professor Kari Rissanen, senior researcher Dr. Juhani Huuskonen and researcher Ph.Lic. Marian Marttina.

1.7 Theory Group, Prof. M. Manninen, Nanoscience Center, Department of Physics, University of Jyväskylä

Prof. M. Manninen (subproject leader), Dr. M. Koskinen, Dr. P. Koskinen, Ph.D. students Thomas Kühn, PhD student Kari Rytkönen.

1.8 Group of Prof. M. Kulomaa, Nanoscience Center, Department of Environmental and Biological Science, University of Jyväskylä

Prof. Markku Kulomaa (subproject leader), Ph.D. students: Dr. Vesa Hytönen (Ph.D. 2005), M.Sc. Teemu Ihalainen. Since 2005, Markku Kulomaa is a professor at the University of Tampere.

1.9 Group of J. Korppi-Tommola, Nanoscience Center, Department of Chemistry, University of Jyväskylä

Prof. Jouko Korppi-Tommola (subproject leader). M.Sc. Ngong Kodiah Beyeh, M.Sc. Jukka Aumanen, M.Sc. Jari Martiskainen (Ph.D. students).

1.11 Funding

Table 1. Funding of the project in 1000 EUR in 2003-2006. Internal funding consists of manpower costs and operational expenditures provided by the organisation. The funding provided by the Academy of Finland and other external sources is also shown in the table.

Partner	Funding organisation	2003	2004	2005	2006	**Total**
P1	Academy	55.20	51.19	52.73	10.88	**170**
P2	Academy	21.35	35.98	41.37	1.30	**100**
P3	Academy	36.63	41.27	38.38	3.72	**120**
P4	Academy	12.49	13.64	23.61	0.26	**50**
P5	Academy	0.70	46.16	33.17	69.97	**150**
P6	Academy	6.64	26.75	26.61	-	**60**
P7	Academy	9.41	26.53	24.06	-	**60**
P8	Academy	-	26.60	13.40	-	**40**
Total		**142.42**	**268.12**	**253.33**	**86,13**	**750**

2 Research Work

2.1 Objectives and Work Plan

The project is divided into three work packages: 1. Bio-nanoelectronics, 2. Molecular electronics based on carbon nanotube rotaxanes, 3. Thermal effects in nanostructures. The objectives for each are:

WP1 Bio-nanoelectronics

Task 1: DNA Detection Sensors (P1,P3,P7,P6)

The objective was to study electrical conductivity of DNA molecules and related sensor applications. Main change from the original plan was to change from the vertical structure to planar electrodes. Significant emphasis in the work has been put on developing controlled methods for trapping single molecules in the nanoscale, and to study the effect of environment e.g. moisture, on DNA conductivity. Single molecule trapping was successfully achieved using metal nanoelectrodes, and the technique was extended towards nanoscale by replacing one of the metal electrodes by a carbon nanotube. In situ confocal imaging of the trapping process was used for studying DNA polarizability.

Task 2: Cell Thermometer (P1, P4)

The objective was to develop nanoscale thermometer for bioapplications. No main changes from the original plan.

WP 2 Molecular electronics based on carbon nanotube rotaxanes (P3, P5, P1, P8, P4, P6)

The objective was to synthesize rotaxanes for functionalizing carbon nanotubes, to develop other functionalizing methods, and study the applicability of the molecules as sensors. No main changes from the original plan.

WP 3 Thermal effects in nanostructures

Task 1. Experimental study of nanofabricated radiation and thermal sensors (P2)

The objective of the work was to study the limiting factor in bolometric radiation sensors: thermal noise. This noise is caused by the exchange of heat between electrons and phonons, i.e. electron-phonon interaction. A further goal listed was studies of low-dimensional samples. Also, we have discovered along the way that virtual photon coupling between nanoscopic metal objects is an important energy relaxation mechanism. This was studied further, meaning less emphasis on the development of the noise measurement technique as outlined in the original plan.

The original objective of the project of the Nanophysics/QE team aims at investigating the electrical and thermal transport properties of single-electron transistors. There are no changes to the objectives listed in the original plan.

Task 2. Theory of electronic properties of nanostructures (P6)

The objective was to study properties of nanostructures, especially thermal effects. No main changes from the original plan.

2.2 Progress Report: Common Themes and Collaboration

The DNA sensor project has been done in a multidisciplinary collaboration.

Controlled manipulation of single molecules is a prerequisite for fully understanding their properties as well as for realizing their potential in molecular electronics. At the present, the fabrication of single-molecule devices in nanoscale mostly relies on passive, uncontrollable methods of manipulation such as deposition of the molecules on the substrate or on the fabricated structure. Dielectrophoresis (DEP), an active manipulation method utilizing electro-magnetic fields, has been widely applied for microscale objects, e.g., λ-DNA. In nanoscale, however, Brownian motion poses a challenge: the few successful demonstrations are for trapping nanoscale objects, and for attaching DNA molecules between nanoelectrodes by DC-DEP. Concerning the intriguing question of DNA conductivity, there starts to be a consensus that dsDNA molecules exposed to untreated SiO_2 or mica surfaces, in dry environment or vacuum, are insulating. However, the conductivity of DNA on specially treated surfaces, in solutions or inside dried films remains open. Also, the effect of humidity on the electrical conductivity of DNA films or constellations of DNA molecules has been discussed recently. The effects of the ambient conditions are related to the intimate connection between the conformation of the molecules and their conductivity.

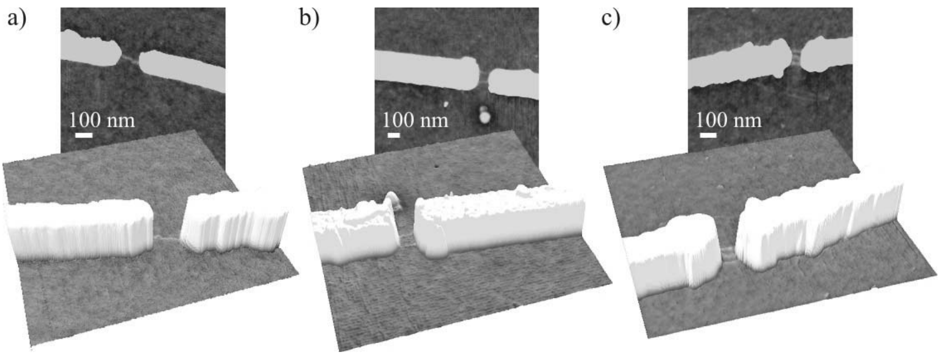

Fig. 1: Atomic force microscope images of one (a), two (b) three (c) DNA molecules trapped by dielectrophoresis between nanoelectrodes fabricated by electron beam lithography [2].

Dielectrophoresis method for trapping and attaching nanoscale dsDNA between nanoelectrodes has been developed in this project. The method gives a high yield of trapping single or a few molecules only which enables transport measurements at the single molecule level. We are the first to demonstrate DC dielectrophoresis (trapping with DC-fields) for nanoscale DNA molecules. The technique is applicable for also other molecules than DNA. For the fabricated samples, electrical conductivity of individual 140 nm long dsDNA molecules was measured, showing insulating behaviour in dry conditions. In contrast, clear enhancement of conductivity was observed in moist conditions, possibly relating to the interplay between the conformation of DNA molecules and their conductivity. The results have been published in [2].

We have extended the trapping technique by using a multiwall carbon nanotube as one of the electrodes. We have shown that the use of carbon nanotube electrodes makes it possible to apply relatively low trapping voltages and still achieve high enough field gradients for trapping nanoscale objects, e.g., single molecules. We compared the efficiency and other characteristics of dielectrophoresis between carbon nanotube electrodes and lithographically fabricated metallic electrodes, in the case of trapping nanoscale DNA molecules. The results were analyzed using finite element method simulations and revealed information about the frequency-dependent polarizability of DNA. The results have been published in [3,58].

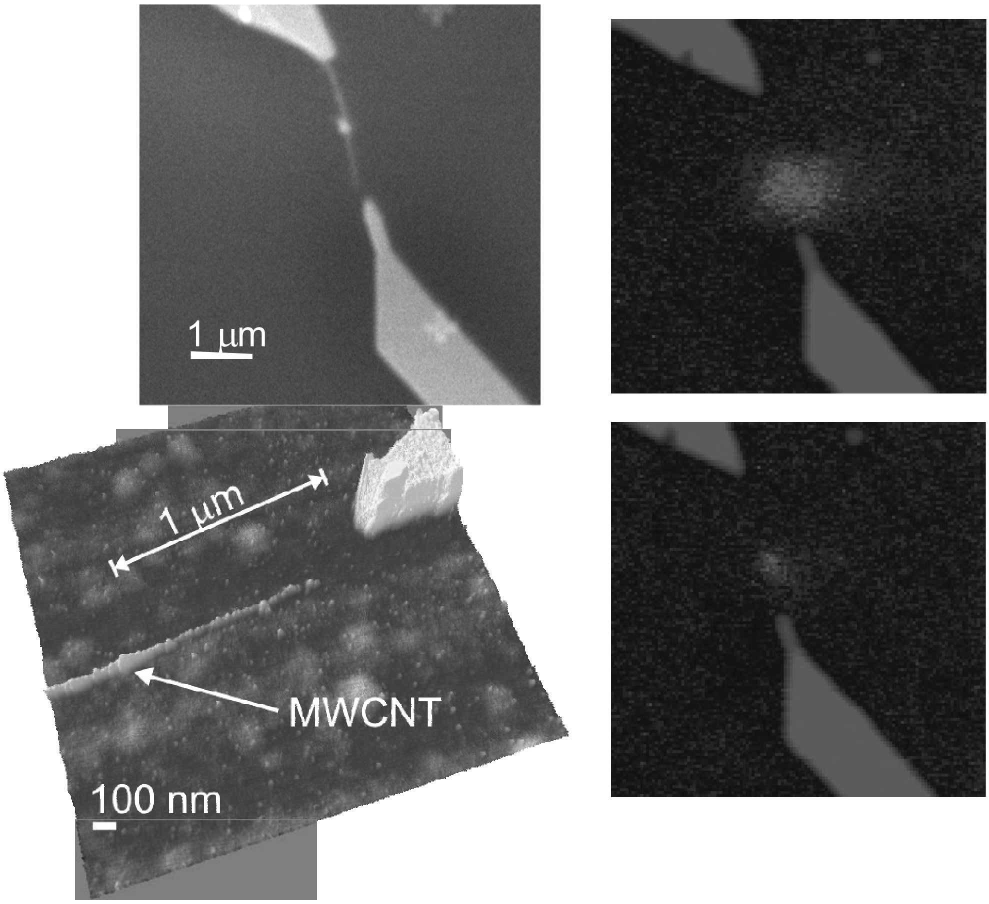

Fig. 2 Dielectrophoresis of 1065 bp dsDNA using CNT as one electrode: SEM (up left) and AFM (down left) images of the multiwalled CNT electrode sample before confocal experiment. The images on the left show the trapped DNA spot when a certain frequency and voltage were used [3].

Another strongly collaborative effort has been the cell thermometer project. A nanoscale thermometer that has the required resolution of 0.1 mK at room temperature has been developed. Results are reported in [4]. Biocompatibility tests have been performed: Silicon nitrate (Si_3N_4), oxidated silicon (SiOxi), evaporated SiO_2 on silicon, Al_2O_3 evaporated on silicon, Ti/Cu/Au layers on Si_3N_4 , Ti/Cu/Au and Ti/Cu/Au + Ti/Al/AlOxi on SiOx, pure gold and ACCUGLASS (Honeywell) on Si_3N_4 were used as platforms for cell cultures. Additionally, methods were developed to enhance or prevent the cell growth on specific chip areas, such as pure gold and silicon monoxide surfaces. Properties of self-assembled monolayers of hexadecanethiol and tri(ethylene glycol) terminated alkanethiol were also studied. Electron lithography was used to control formation of the monolayers of surface materials and the biocompatibility was further assessed by comparing NLFK-cell growth on control surfaces (Nunc cell culture dishes) and the manufactured surfaces by imaging the cells after one and two days in normal cell culture conditions.

The project on rotaxane-functionalized carbon nanotubes was also collaborative, however, consecqutive phases of the work were done by different groups, therefore the results are presented below, in the progress reports of the individual groups.

The collaborative aspect was strong also in the theory work, because it was to large extent closely related to the experiments done within the project. A numerical algorithm was developed which can calculate the exact phonon modes of thin membranes based on full elasticity theory. Using this code intriguing results on ballistic phonon transport have been achieved, spanning the whole range from fully 3D substrate to fully 2D phonon system. Due to the increase of the phonon density of states at low energies when the membrane thickness is reduced, we have obtained a counter-intuitive result: the thermal conductance can increase with decreasing thickness. This can have wide implications for the design of optimal X-ray sensors for space and terrestrial applications. Calculation of electron-phonon interaction in 2D membranes has also been done.

2.3 Progress Report: Progress by the Nanoelectronics group (P1)

All the work by P1 was strongly collaborative and has been described above (the trapping and DNA project, and the cell thermometer project).

2.4 Progress Report: Progress by the Experimental Nanophysics group (P2.1)

Summary

We have used symmetric normal metal-insulator-superconductor (NIS) tunnel junction pairs, known as SINIS structures, for ultrasensitive thermometry in the temperature range 50 - 700 mK. By Joule heating the electron gas and measuring the electron temperature, we have shown that the electron-phonon (e-p) scattering rate in the simplest noble metal disordered thin films (Cu, Au) and more complex films of Al doped with Mn can be tuned by the level of disorder. Specifically, the AlMn films follow a T^4 temperature dependence, leading to a stronger decoupling of the electron gas from the lattice at the lowest temperatures. This power law is indicative e-p coupling mediated by vibrating disorder, in contrast to the previously observed T^3 and T^2 laws. Our result has several practical consequences. Compared to a lower power dependence, it is harder to cool the electrons with cold phonons. Direct electron cooling then becomes more important. On the other hand, a sensor based on the hot electron effect is even more sensitive, since the ultimate noise equivalent power of such a detector is proportional to the square root of the thermal conductance. In addition, we have also developed an ac-technique to measure the electron-phonon (e-p) scattering rate directly, without any other material or geometry dependent parameters, based on overheating the electron gas. The technique is based on Joule heating the electrons in the frequency range DC-10 MHz, and measuring the electron temperature in DC.

Because of the nonlinearity of the electron-phonon coupling with respect to temperature, even the DC response will be affected, when the heating frequency reaches the natural cut-off determined by the e-p scattering rate. Results are in agreement with indirect measurement of similar samples and numerical modeling of the non-linear response.

Detailed report

Although the interaction between conduction electrons and thermal phonons is elementary for many processes and phenomena at low temperatures, there are still relatively few experimental studies that conclusively support the theoretical description, particularly for typical disordered thin film samples. Several earlier results indicated that even for disordered films, the temperature dependence for the electron-phonon (e-p) scattering rate follows the power law expected for pure samples with coupling to longitudinal phonons only: $1/\tau \sim T^3$ [61,62]. These results confirmed the relation $P=\Sigma\Omega \ (T_e^5-T_p^5)$ between heating power P and electron and phonon temperatures T_e and T_p in a volume Ω and it is widely used for thin film metallic samples at low temperatures. However, the theory [63] for disordered thin films predicts that the scattering rate from vibrating disorder (impurities, boundaries etc.) is $1/\tau \sim T^4$ in the limit $ql < 1$, where q is the wavevector of the dominant thermal phonons and l the electron mean free path. This leads to the relation $P=\Sigma\Omega \ (T_e^6-T_p^6)$, a result that has not been widely confirmed. In fact, we are not aware of any observation of it in standard normal metal films like Cu, Al, Au etc.

In this project we report the observation of the disorder-weakened electron-phonon (e-p) scattering in evaporated Cu,Au and AlMn thin films [6,8,9,10,11]. We have measured the rate at which electrons in a normal metal wire overheat, when DC power is applied to it by Joule heating, at sub-Kelvin temperatures. This technique has been shown to give the energy-loss rate directly, in contrast to the temperature dependence of the weak localization resistance, which gives the dephasing rate. The overheating rate is determined by measuring the electron temperature T_e directly with the help of symmetric normal metal-insulator-superconductor (NIS) tunnel junction pairs, known as SINIS structures. SINIS-thermometers have been shown to be extremely sensitive thermometers, operating at the lowest experimentally achievable temperatures. Therefore, they are also candidates for ultrasensitive microbolometers in the sub-Kelvin temperature range.

Our result has several practical consequences. Compared to a lower power dependence, it is harder to cool the electrons with cold phonons. Direct electron cooling then becomes more important. On the other hand, a sensor based on the hot electron effect is even more sensitive, since the ultimate noise equivalent power of such a detector is proportional to the square root of the thermal conductance. Also, for AlMn, the strength of the e-p interaction was shown to be tunable by the concentration of Mn Kondo ions in the Al matrix, giving a novel way to tune the interaction by choosing the concentration.

In addition, we have also developed an ac-technique [7,32] to measure any thermal relaxation rate directly, without any other material or geometry dependent parameters, based on overheating the electron gas. The technique is based on Joule heating the electrons in the frequency range DC-10 MHz, and measuring the electron temperature in DC [5]. Because of the nonlinearity of the electron-phonon coupling with respect to temperature, even the DC response will be affected, when the heating frequency reaches the natural cut-off determined by the e-p scattering rate. Results are in agreement with indirect measurement of similar samples and numerical modeling of the non-linear response.

Another observation during this project was that the properties of tunnel junctions that are used for thermometry can be improved and stabilized by vacuum annealing techniques [59,33]. This is an obvious advantage, when considering practical and commercial applications of tunnel junction devices. One possible application for the annealing is to increase the sensitivity of Josephson junction threshold current detectors, currently used for example in superconducting quantum bit readouts or in shot-noise measurements.

We have also discovered during this project that thermal conduction due to near field photons can be a significant process at low temperatures in nanostructures [34]. Work is ongoing to clarify these issues.

Finally, theoretical work on phonon transport in ballistic 2D systems showed a curious phenomenon: The heat conductance of a thin membrane can be improved by *decreasing* the thickness of the membrane [12]. This is significant for the operation of thermal detectors.

2.5 Progress Report: Progress by the Nanophysics/QE team

Theory of transport in superconducting single-electron transistors and other mesoscopic structures: We have been simulating electric and thermal quasiparticle transport processes in single-electron transistors. The master equation within the so-called orthodox theory is solved numerically for experimentally relevant values of superconducting gap, temperature, and charging energy. We have also investigated the macroscopic quantum-mechanical description of a running-phase state in a Josephson junction.

Experimental results on single-electron transistors: We have designed, fabricated and measured a single-electron Al transistor in which the island is not in contact with the substrate (see Fig. 1). The measurements indicate that good functional devices can be fabricated by simply etching away the substrate. The structure was remarkably robust, surviving several cooldowns. The merit of this device is that – by fabrication- it will allow further studies on the relative importance of different sources of 1/f noise (e.g. intrinsic noise of the junctions vs. substrate noise). For the problem of heating/cooling effects in SET's, this structure allows the elimination of the leak heat into the substrate; if similar structures are used as coolers, the thermal decoupling of the substrate is beneficial.

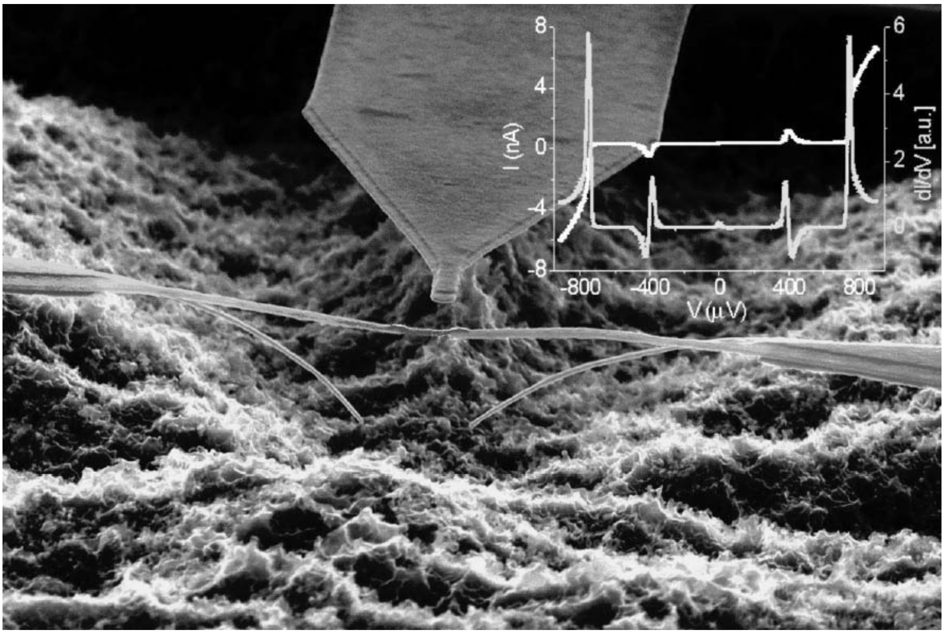

Fig. 3: Colorized SEM picture of an all-Al superconducting suspended SET. The island (red) floats above the substrate and it is in contact trough tunnelling junctions only with the left and right electrodes. Inset (right up): IV characteristics showing typical transport processes in these structures (Josephson tunnelling, JQP, and quasiparticle tunnelling). The picture is from the publication [16], and was chosen to be the cover picture of the corresponding Applied Physics Letters issue; it was further republished in the American Institute of Physics Report 2005.

Interaction-free measurement with superconducting circuits.

We have proposed an interaction-free measurement protocol for a quantum circuit consisting of a superconducting qubit and a read-out Josephson junction. By measuring the state of the qubit can ascertain the presence of a small pulse of electric current without any disturbance due to energy exchange with the continuum of states outside the washoard potential well in which the qubit is localized. An experiment of this type would constitute a test, at the macroscopic level, of a strongly nonclasical consequence of quantum mechanics. Two fundamental physical processes, interferometry and tunneling, are combined here to demonstrate the equivalent of the optical Mach-Zender interaction-free detection scheme for this superconducting quantum circuit. The crossover between standard interference effects (such as the shift in the interference pattern due to phase difference accumulated) and the interaction-free phenomenon is also discussed.

The results have been published in [17,18,20].

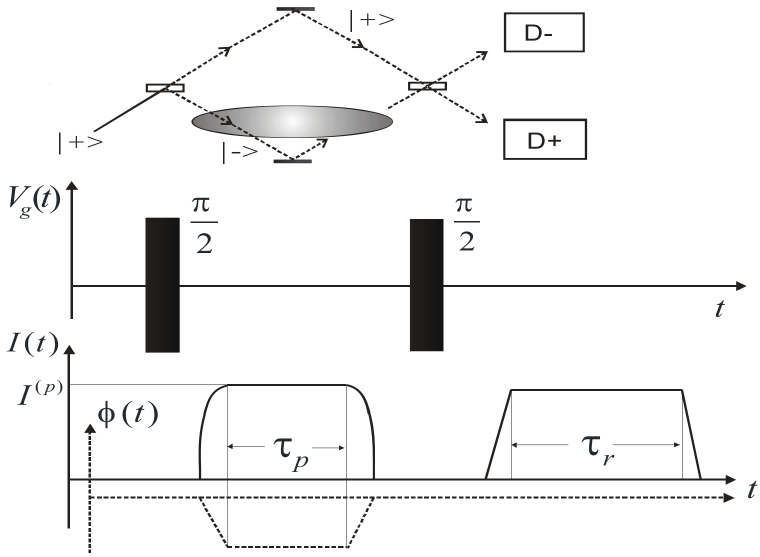

Fig. 4 Mach-Zehnder interferometric setup **(**upper schematic**)** and the Quantronium pulse sequence **(**graphs below**)** with the axes of the flux graph slightly displaced for clarity.

Microwave-induced coupling of superconducting qubits

We investigate theoretically the quantum dynamics of a system of two coupled superconducting qubits under microwave irradiation. We find that, with the qubits operated at the charge co-degeneracy point, the quantum evolution of the system can be described by a new effective Hamiltonian which has the form of two coupled qubits with tunable coupling between them. This Hamiltonian can be used for experimental tests on macroscopic entanglement and for implementing quantum gates.

The results have been published in [19].

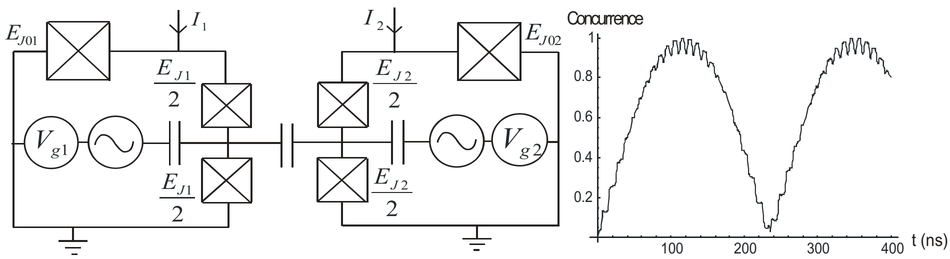

Fig. 5 Schematic of the capacitive coupling between two mixed charge-flux qubits and a graph showing the calculated concurrence for the case of relatively large equal-amplitude microwave coupling to each of the qubits, proving that the qubits become entangled.

2.7 Progress Report: Progress by the group of J. Virtanen (P3)

Purification and Chemical Functionalization of Carbon Nanotubes
In order to use carbon nanotubes (CNT) in advanced applications, such as electronics and sensors, they mush be coupled with each other, nanoparticles, or molecules. Prerequisite is to attach functional groups or moieties. We have developed new functionalization methods. Our method can be combined with magnetic purification so that essentially in one step the CNTs can be purified and functionalized. Functional groups that have been attached onto the CNTs so far include amino and thiol groups. These allow binding of a myriad of organic and biomolecules as well as nanoparticles with the CNTs. Preliminary measurements indicate that our modification methods have not harmed the electrical conductivity of the CNTs. The electrical measurements were done in collaboration with P1.

So far we have filed four patent applications to protect these methods, and the spin-off company Nanolabsystems has been founded. It has proceeded its research and development further within the Nanoscience Center facilities for start-up companies. The company web-page: [64].

2.8 Progress Report: Progress by the group of M. Vuento (P4)

The work was strongly collaborative and has been reported above (the cell thermometer project). In addition to the electronic cell thermometer, principle of a novel scheme for electro-optical micro/nanoscale temperature measurement was tested, based on fluorescent detection of phase transitions in model membranes. The fluorescent detection was based on different spectral properties of di-4-ANEPPDHQ, previously known as a probe for membrane potential, when bound to differently organized lipid phases. Depending of membrane composition, changes in quantum yield and emission peak position were detected within a temperature range of 5oC-40oC, suggesting that an optical nanoelectronic device might be constructed for temperature measurement covering this range. At a later stage of the research, we studied phase distribution in lipids of intracellular membranes of NLFK cells.

2.9 Progress Report: Progress by the Organic Chemistry Laboratory (P5)

The target of the Rissanen group in WP2 was to prepare a CNT-rotaxane in collaboration with the Virtanen group. Virtanen group has focused on the purification of the CNT's while the Rissanen group has been responsible for the synthesis chemistry of the "wheel" molecules needed in the final CNT-rotaxane. Figure 1 depicts the schematic structure of the CNT-rotaxane (Fig. 6 A and B). Into a 5 – 10 nm long CNT a photoactive macrocycle is non-covalently attached. Photoexitation of the macrocycle will affect the electrical properties of the CNT leading to measurable sensor behaviour. The CNT-rotaxane is a truly innovative and extremely ambitious goal. During the three years hard work it turned out that this final goal could not be reached. The CNT purification turned out to be very demanding and even though some succees was achived, no CNT samples suitable (5 – 10 nm long pure CNT's) could not be obtained during this project. The final assembly of the CNT-rotaxane was to be achieved via self-assembly of the suitable macrocycle (some target macrocycles are presented in figure 6, GS1a and GS 10a) with the CNT with so called "slipping" method.

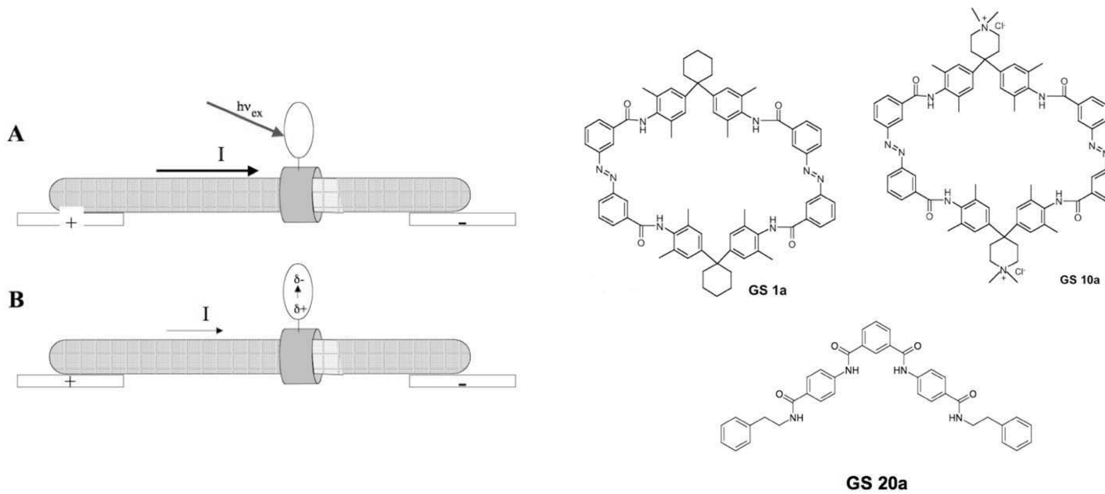

Fig. 6 The schematic presentation of the CNT-rotaxane (A and B) and a few target macrocyles (GS 1a and 10a) and a clip molecule (GS 20a).

The synthesis of the macrocyles and later "clip" (see below) molecules required for the carbon nanotube (CNT) rotaxane were excetuted. The first approach for these functional macrocycles utilized the earlier knowledge on the piperazinophanes, large macrocycles consisting of piperazine and suitable aromatic spacers with photoactive groups. The synthesis of these piperazinophane requires lacrymatic alkyl bis-bromides as starting material. During the synthesis work the researcher was exposed to these bis-bromides, which was, after some months, manifested by severe allergic reactions. These allergic reactions were so severe that they required a medical attention and to remove these health problems, complete exclusion of alkyl bis-bromides had to be adopted. Since the macrocycles were not complete at this state of the project all the previous results utilizing bis-bromides had to be abandoned and a new strategy had to be taken. The first new macrocyclization attempt focused on the use of Schiff base macrocycles, after seven months work it came evident that also this line of research did not produce the desired macrocycles. Since March 2005 a third method of macrocycle synthesis was started, now using bis-amines and bis-acid chlorides, leading to rigid amide-macrocycles (Fig. 6, GS 1a and 10a). The bis-amine and bis-acid chloride building blocks needed for the final large enough macrocycles were much easier to prepare. The synthesis of the building blocks succeeded well but the final cyclisation leading to macrocyclic amides were not successful. Some macrocycles in very impure form was obtained, but the very time-consuming purification of the macrocycle mixtures turned out to be unsuccessful. Due to the severe difficulties in the cyclization reactions, an alternative route was taken in the final eight months of the project. Instead of slipping of a macrocyle into the CNT the photoactive moiety can be attached in to CNT by pi-pi interactions of a suitably curved molecule. These "clip" molecules are much easier to prepare and should be robust enough to act as the slipped macrocycles. The last eight months of the project (until December 2006) synthesis work was focused on these clip molecules. Due to the ending of the project the clip molecules could not be tested with CNTs.

One publication [21] and three patent applications [65,66,67] were produced related to the synthesis work done in this project.

2.10 Progress Report: Theory Group (P6)

The electronic structure and magnetic properties of quantum dots and rings have been studied using the density functional method and exact diagonalization techniques. A multicomponent density functional model has been developed to deal with multiwalley semiconductors and vertical double dots. The results indicate increased tendency of electron localization with increasing number of internal degrees of freedom of the electron system.

The magnetic properties of quantum dot arrays were studied using local spin-density approximation. We predicted that properly constructed rows of quantum dots can be used as tunable spin-filters for spintronics applications.

Exact diagonalization techniques have been used to study persistent currents in quantum rings and vortex formation in quantum dots. The main emphasis was put on the use of spectral information for explaining the complicated rotational states caused by an external magnetic field. We found that the periodicity of the persistent current of a ring depends on material parameters like effective Lande factor. For quantum dots in magnetic fields we showed that the vortex formation can be understood with help of electron-hole duality and can be detected by use of tunneling spectroscopy.

The electronic structure of carbon nanotubes surrounded by rotaxane molecules were studied using Car-Parrinello method in order to study their applicability as molecular sensors. Pseudorotaxane systems based on crown ethers or β-cyclodextrin and single walled carbon nanotubes were studied. It was observed that it was necessary to link the molecule chemically to the nanotube in order to change its conductance via the sensor molecule.

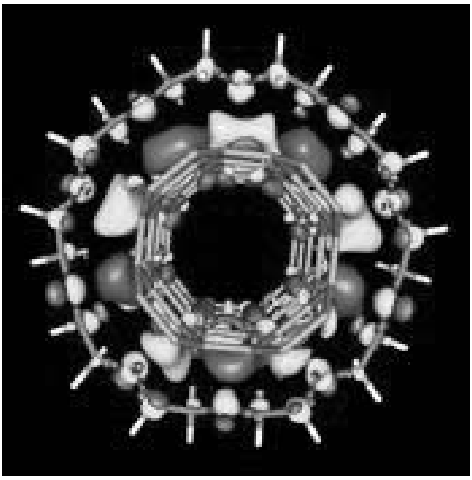

Fig. 7 Rotaxane molecule around a carbon nanotube showing the highest occupied electron orbital [39].

2.11 Progress Report: Progress by the group of M. Kulomaa (P7)

The work was strongly collaborative and has been reported above (the DNA and trapping project).

2.12 Progress Report: Progress by the group of J. Korppi-Tommola (P8)

Spectroscopic and energy transfer properties of light sensitive supramolecular complexes

Two supramolecular families with dansyl fluorescent labels were studied by using absorption and fluorescence spectroscopy and femtosecond time resolved measurements. The new supramolecules were partly synthesized by partner 5 (resorcinarenes) of the consortium and partly obtained from the University of Bonn (Prof. F. Vögtle). Besides excitation energy transfer properties in synthetised supramolecular structures in-vivo light harvesting antenna systems of photosynthetic bacteria were studied especially rod-like antenna assemblies of bacteriochorophyll c of green bacteria. Experiments with the dye bound carbon nanotubes, prepared by partner 3, are still in progress. For excitation in the UV region an optical setup to produce about 100 fs UV pulses was built. Home built tunable NOPAs were used for probing in the visible region.

One of the aims of the work was to design supramolecular structures complexed with acceptor molecules, in such a way that UV excitation energy would be transferred spatially in the supramolecule and excitation released as emission in the visible spectral region. Such complexes imbedded in polymer matrix have a potential serve as sensitive and cheap UV sensors. So far the best working system studied was dansylated POPAM dendrimer generations of G2, G3 and G4 containing 8, 16 and 32 dansyl groups, respectively complexed with the fluorescent dye, eosin. Below are shown some results for this system. (Fig.8)

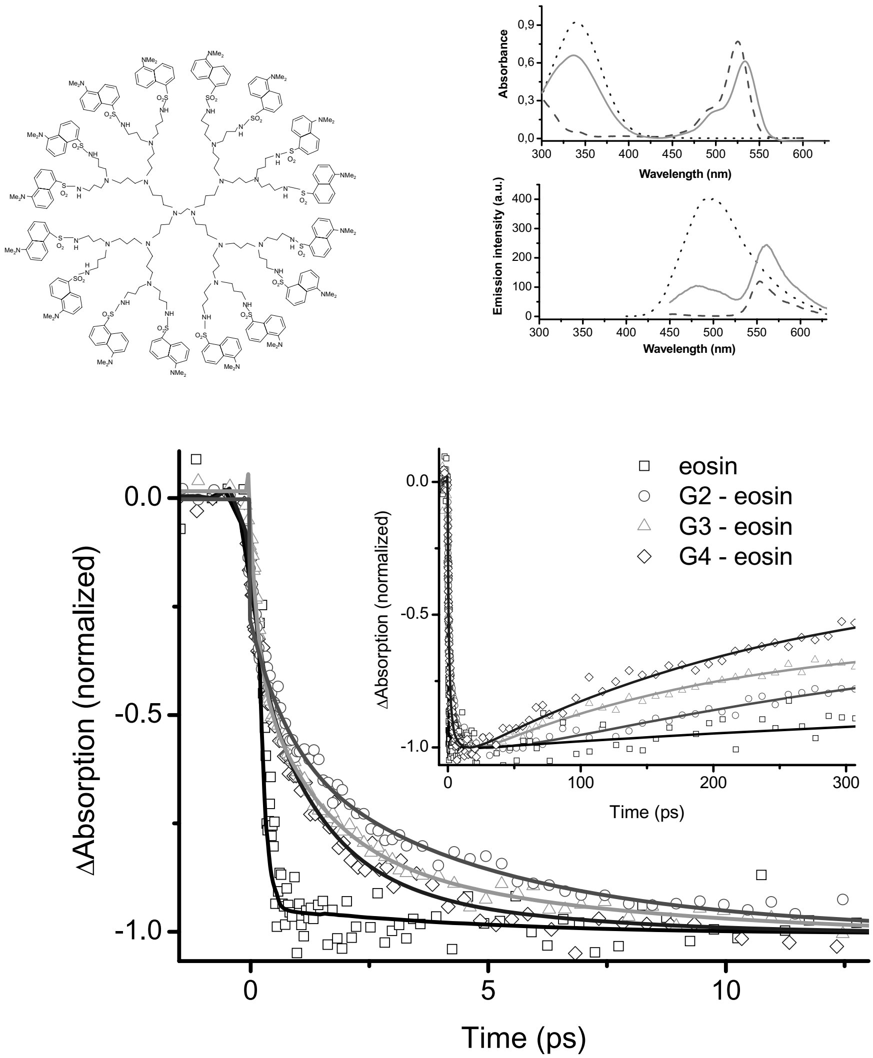

Fig. 8 Absorption and fluorescence spectra of dansylated G3 POPAM (blue), eosin (red) and the complex (green, TOP RIGHT), bleach recovery of eosin and the G2, G3 and G4 complexes at 560 nm after 100 fs excitation at 340 nm showing excitation energy transfer from the dansyl chromophores to the eosins (BOTTOM), schematic structure of the G3 – dansylated POPAM complex (TOP LEFT).

In the study eosin – dendrimer and eosin - eosin interactions in the complexed supramolecular structure could be identified and visible emission from dansyls seen after UV excitation. The results suggest that the esosin(s) is(are) bound via hydrogen bonding in the dansyl periphery of all supramolecules studied and not in the center region [28]. Study of emission lifetimes and anisotropies of the complexes was carried out at the University of Lund. A manuscript of these results is in preparation.

The second group of dansylated supramolecules studied belongs to resorcarene family. For a reference compound monosubstituted dansyl, phenyldansyl sulphonate was prepared. The strongest emission of the series of these compounds was found from the monosubstituted dansyl followed by weaker emission of dansyl substituted resorcarenes with 4 and 8 dansyls. Femtosecond streak camera measurements of these compounds will be carried out in the spring 2007. It was shown that protonation of dansyls quenched the emission of all labeled supramoleculer complexes efficiently [69].

Bacteriochlorophyll c molecules form tubular J-type aggregates containing thousands of pigments. Such aggregates serve as building blocks to internal pigment organization of in-vivo antenna, chlorosomes of green bacteria containing up to 300 000 pigment molecules. Extensive studies of such systems were carried out to unravel how excitation energy flows in such complicated assemblies of pigments that are able to capture light under extremely low light conditions like at the bottom of a lake. It is hoped that such studies help understanding excitation energy transfer in self assembled molecular aggregates that show promise as lossless nanoscale waveguides. It was shown that energy transfer in stacked rod structures takes place in about 200 fs across the long axis of the chlorosome after which energy is transferred in picoseconds to the much lower density pigment assemblies in the baseplate of the chlorosomes. Two manuscripts an experimental [70] and a theoretical (in preparation) have been written on these results. An invited article on excitation energy transfer in assemblies of photosynthetic pigments was published in January 2006 as a cover story of *Phys.Chem.Chem.Phys* [29].

3 International Aspects

The project is closely related to several EU-funded projects: The Nanophysics/QE team has been part of the QIPC EU network, and of the SQUBIT and SQUBIT-2 projects of the European Union. M. Manninen is the coordinator of the ULTRA-1D (NMP4-CT-2003-505457) project of the European Union. P. Törmä and S. Paraoanu participate in the QUROPE (contract number 033622) Coordination Action in the IST programme of the European Union.

International collaboration with professor Fritz Vögtle (macrocycle synthesis) and Dr. Christoph Shalley (mass spectrometry) Kekule Institut fuer Organische Chemie und Biochemie der Universität Bonn, Germany. Recently collaboration with professor Jean-Pierre Sauvage, University of Strasbourg, France on related macrocycle synthesis was started. Kari Rissanen (P5) is actively participating in ESF COST programmes from 1995 up to date. A COST working group in COST D31 “Organising Chemical Systems with Selected Functions” was approved February 2005, this WG consists of eight research groups (Italy, Finland, Germany, Belgium, 2 x Portugal and 2 x Spain).

In WP3, the theoretical work on thermal transport, there is a group at Oslo University (Prof. Galperin, Dr. Anghel) who are directly involved. Experimentally, collaboration has just started with two institutions providing novel materials for the study of thermal properties: at Indian Institute of Technology Kanpur (prof. Budhani) and at University of California at Santa Barbara (prof. Cleland). In addition, we are directly involved in

ESA funded projects developing thermal detectors, one in collaboration with Oxford Instruments Analytical company, and another one in collaboration with the Space research Organization Netherlands (SRON). The research of the theory group is done in international collaboration with Lund Institute of Technology, University of Oslo, Nordita, and Bose Center in Calcutta.

In WP2 two important international co-operations were realized. The dansylated POPAM dendrimers for this work were obtained from the University of Bonn (Prof. F. Vögtle) and the fluorescence streak camera measurements not accessible in Jyväskylä were carried out at the University of Lund (Prof. Villy Sundström).

All results will and have been publicized at international conferences and in research journals. Several research visits abroad have been arranged, as well as visits of foreign researchers to Jyväskylä.

4 Publications and Academic Degrees

Partner	Type of publication	2003	2004	2005	2006	**Total**	Publication numbers
P1	Ref. journal art.	-	-	2	2	**4**	1-4
	Ref. conf. papers	1	-	-	-	**1**	30
	Monographs	-	-	-	-	**-**	
	Doctoral dissert.	-	-	-	1	**1**	37
	Licentiate degrees	-	-	-	-	**-**	
	Master degrees	-	1	2	1	**4**	42-45
P2.1	Ref. journal art.	1	2	1	6	**10**	5-14
	Ref. conf. papers	-	1	-	3	**4**	31-34
	Monographs	-	-	-	-	**-**	
	Doctoral dissert.	-	-	-	1	**1**	38
	Licentiate degrees	-	-	-	-	**-**	
	Master degrees	2	-	1	2	**5**	46-50
P2.2	Ref. journal art.	-	-	3	3	**6**	15-20
	Ref. conf. papers	1	-	-	-	**1**	35
	Monographs	-	-	-	-	**-**	
	Doctoral dissert.	-	-	-	-	**-**	
	Licentiate degrees	-	-	-	-	**-**	
	Master degrees	-	-	1	2	**3**	51-53

P3	Ref. journal art.	-	-	-	-	**-**	
	Ref. conf. papers	-	-	-	-	**-**	
	Spin-off companies	-	1	-	-	**1**	64
	Doctoral dissert.	-	-	-	-	**-**	
	Licentiate degrees	-	-	-	-	**-**	
	Master degrees	-	1	-	-	**1**	54
P4	Ref. journal art.	-	-	-	-	**-**	
	Ref. conf. papers	-	-	-	-	**-**	
	Monographs	-	-	-	-	**-**	
	Doctoral dissert.	-	-	-	-	**-**	
	Licentiate degrees	-	-	-	-	**-**	
	Master degrees	-	-	-	-	**-**	
P5	Ref. journal art.	-	-	-	1	**1**	21
	Ref. conf. papers	-	-	-	-	**-**	
	Monographs	-	-	-	-	**-**	
	Doctoral dissert.	-	-	-	-	**-**	
	Licentiate degrees	-	-	-	-	**-**	
	Master degrees	-	1	-	-	**1**	55
P6	Ref. journal art.	-	4	1	-	**5**	22-26
	Ref. conf. papers	1	-	-	-	**1**	36
	Monographs	-	-	-	-	**-**	
	Doctoral dissert.	-	-	-	1	**1**	39
	Licentiate degrees	-	-	-	-	**-**	
	Master degrees	-	-	-	-	**-**	
P7	Ref. journal art.	-	-	1	1	**2**	1,21
	Ref. conf. papers	1	-	-	-	**1**	30
	Monographs	-	-	-	-	**-**	

	Doctoral dissert.	-	-	1	-	**1**	40
	Licentiate degrees	-	-	-	-	**-**	
	Master degrees	-	-	1	-	**1**	56
P8	Ref. journal art.	-	1	-	2	**3**	27-29
	Ref. conf. papers	-	-	-	-	**-**	
	Monographs	-	-	-	-	**-**	
	Doctoral dissert.	-	-	-	1	**1**	41
	Licentiate degrees	-	-	-	-	**-**	
	Master degrees	-	1	-	1	**2**	57-58

5 Other Activities

The steering activities included monthly meetings of the whole consortium, arranged in connection of the monthly meetings of the Nanoscience Center steering committee. In individual collaborative projects, discussions took place in a weekly or daily basis. The collaborative research was strongly enhanced by the move to the new, common Nanoscience Center in August 2004.

Dr. Maasilta was a member of the organizing committee of the Jyväskylä Summer School in 2004 and a vice-chair in 2005.

Seminars reporting on research activity done within the consortium have been arranged within the NanoPhysics Seminar series at the University of Jyväskylä.

Nanoscience has been strongly publicized by the Nanoscience Center: hundreds of people have visited the Nanoscience Center since its opening 2004, and the outreach programme includes also lectures by the professors in the local schools.

A yearly Jyväskylä Nanoscience Seminar has been established, the first one in 2004 featured leading scientists in the field such as Prof. Sumio Iijima, the inventor of carbon nanotubes. The event gathers audience from all over Finland, and has been established organized also in 2005 and 2006, and will be continued as a yearly event.

The participants of this consortium and the Nanoscience Center at the University of Jyväskylä in general have played an important role in developing the national nanoscience initiative. The strongly collaborative Nanosensors project reported here has been essential in establishing the contacts, collaborations and multidisciplinary view point enabling also our activity at the national level in nanosciences.

Two Nordforsk workshops were arranged in the Nanoscience center in Jyväskylä: Quantum Properties of Nanostructures, October 2005 and Low-Dimensional Physics: The Theoretical Basis of Nanotechnology, October 2006.

6 Publications

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ROOM TEMPERATURE SPINTRONICS (SPIN)

Markku Sopanen[1], Pekka Kuivalainen[2], Filip Tuomisto[3] (Kimmo Saarinen), and Jouni Ahopelto[4]

Abstract

The main objective of the research in this consortium was to produce III-V semiconductor material having ferromagnetic properties at room temperature. In this aspect the consortium has been successful. Electron Physics Group, TKK, has fabricated GaMnN material with Curie temperature of 330K. Also GaMnAs and InMnAs layers and structures have been fabricated by metalorganic vapor phase epitaxy and molecular beam epitaxy. Defect properties of GaMnAs and ZnMnO have been studied. Magnetic resonance tunnelling diodes and magnetic Zener diodes have been fabricated and investigated. Magnetic semiconductor-superconductor junctions and energy transport between hole gas and crystal lattice have been studied at sub-kelvin tempratures.

1 Partners and Funding

1.1 Optoelectronics Group (OEG), Micro and Nanosciences Laboratory, Helsinki University of Technology (TKK)

The research group consists of docent Markku Sopanen and graduate students Hannu Koskenvaara, Pasi Kostamo, Teemu Lang, Tapio Rangel, Outi Reentilä, Juha Riikonen, Jaakko Sormunen, Sami Suihkonen, Olli Svensk, and Pekka Törmä.

1.2 Electron Physics Group (EPG), Micro and Nanosciences Laboratory, Helsinki University of Technology (TKK)

The research group in spintronics consists of professor Pekka Kuivalainen, senior research scientist Sergey Novikov and graduate students Heikki Holmberg and Natalia Lebedeva.

1.3 Positron Research Group, Laboratory of Physics (LP), Helsinki University of Technology (TKK)

The research group consists of subproject leader docent Filip Tuomisto, senior researchers docent Jonatan Slotte and Dr. Asier Zubiaga, and graduate students Simo Kilpeläinen, Katja Kuitunen, Jussi-Matti Mäki, Antti Pelli, Floris Reurings, Mikko

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Rummukainen, and Petri Sane. The group also employs two undergraduate students. The group was headed by prof. Kimmo Saarinen until the end of 2005.

1.4 VTT Micro and Nanoelectronics (VTT)

The research group consists of research professor Jouni Ahopelto, Dr. Jani Kivioja, and graduate students Tomi Haatainen and Mika Prunnila.

1.5 Funding

Table 1. Funding of the project in 1000 EUR in 2003-2006. Internal funding consists of manpower costs and operational expenditures provided by the organisation. The funding provided by the Academy of Finland and other external sources is also shown in the table.

Partner	Funding organisation	2003	2004	2005	2006	**Total**
OEG, TKK	TKK	30	50	50	30	**160**
	Academy	28	57	55	27	**167**
EPG, TKK	TKK	5	20	20	5	**50**
	Academy	22	45	45	21	**133**
LP, TKK	TKK	25	25	25	25	**100**
	Academy	22	47	53	1	**123**
VTT	VTT	13	25	40	30	**108**
	Academy	30	35	70	37	**172**
Total		**175**	**304**	**358**	**176**	**1013**

2 Research Work

2.1 Objectives and Work Plan

The objectives of the Optoelectronics Group, TKK were as follows: "the main objective of the research is to produce III-V semiconductor material having ferromagnetic properties at room temperature. The main effort is directed to the growth of device quality GaMnN layers primarily by MOVPE. Alternative approach is to grow GaN layers by MOVPE at OEG and use Mn diffusion to form GaMnN in the MBE chamber at EPG."

The objectives of the Electron Physics Group, TKK, were: (i) to grow room temperature ferromagnets of Mn-doped GaN by using solid state diffusion, (ii) to characterize the electrical and magnetic properties of the grown samples in order to determine, e.g., the dominant transport mechanism and Curie temperature, (iii) to fabricate spintronic semiconductor devices such as magnetic tunnelling diodes, resonant tunnelling devices and pn-junctions both of Mn-doped GaAs and GaN.

The objectives of Positron Research Group, TKK, were: (i) to study the compensation of Mn in both GaMnAs and GaMnN alloys, (ii) to investigate diffusion of Mn and clustering of Mn and the relation of these effects to the magnetic properties in GaMnN and GaMnAs, and (iii) to perform positron annihilation studies to learn of the optimal growth conditions for GaMnN and nitride semiconductors in more general.

The objective of the Nanoelectronics group, VTT, was to fabricate and investigate superconductor-ferromagnetic semiconductor tunnel junctions. These junctions form a new field of interesting basic physics and have high potential for realisation of high efficiency electronic microcoolers. Another objective is to perform materials characterisation at low temperatures and high magnetic fields.

2.2 Progress Report: Common Themes and Collaboration

Collaboration in the consortium has been extensive. OEG has provided samples for EPG and LP. EPG has provided material for LP and VTT. Many samples and sample series have been planned together with the participating groups.

One area of active cooperation has been the fabrication of magnetic semiconductors and their structures in the consortium. Due to the severe memory effects attained while using manganese in the MOVPE system at OEG, alternative methods to fabricate magnetic semiconductors had to be devised. One approach has been the diffusion of Mn into the host semiconductor in the MBE chamber at EPG. OEG has supplied GaAs, GaN, InN layers and nearly complete resonance tunnelling diode structures from AlAs/GaAs material system for EPG for further processing and studies.

One major common theme has been to study point defects and defect complexes in magnetic semiconductors, and their role in the magnetic properties. Samples fabricated at OEG and EPG have been supplied for LP for positron and infrared absorption studies. In addition to the magnetic samples a lot of effort has been made in the fabrication and research of the host materials. To understand the defect properties of GaMnAs and GaMnN also the defect structure of GaAs and GaN has to be understood.

EPG has also fabricated GaMnAs material and device structures for VTT for sub-kelvin measurements and magnetic semiconductor-superconductor junction studies.

2.3 Final Report: Optoelectronics Group (OEG), Micro and Nanosciences Laboratory, Helsinki University of Technology (TKK)

One objective of OEG was to fabricate GaMnAs, InMnAs and GaMnN layers by metalorganic vapour phase epitaxy. During the first studies a severe memory effect of manganese was observed. For example, test samples of GaAs on GaAs were grown after a series of MnGaAs samples. XRD measurements showed Mn incorporation of about 0.05 % even after susceptor and reactor bake sequences were completed. The Mn concentration was observed to decrease when Mn was not used in the reactor for months. Due to this contamination problem some plans were changed and, e.g., GaMnN was not grown by MOVPE in this project.

However, GaMnAs and InMnAs were grown by MOVPE. The highest Mn incorporation observed in MnGaAs was 5.0 %. The surface morphology of most of the MnGaAs samples was good, almost atomically flat. Photoluminescence measurements of MnGaAs at 10 K showed (Fig. 1), besides the normal GaAs excitonic luminescence peaks around 1.5 eV, deep-level luminescence at around 1.4 eV. These peaks have been attributed in literature to Mn acceptor transitions, and they were most clearly seen in samples with less than 1 % of Mn. In samples with larger Mn concentration, the luminescence intensity dropped drastically. Donor-acceptor pair (DAP) or free-to-bound (FB) luminescence was observed up to Mn concentration of 2.8 %. For MnInAs, Mn incorporations of up to 0.9 % were achieved. MnInAs surfaces had more features, such as small holes, dots, and clusters.

In addition to the growth studies of GaMnAs and InMnAs, OEG delivered material (layers and device structures) made of InN, GaN and GaAs-based materials for the other groups (see e.g. Fig. 7). For example, EPG diffused Mn into InN samples, but ferromagnetism was not observed.

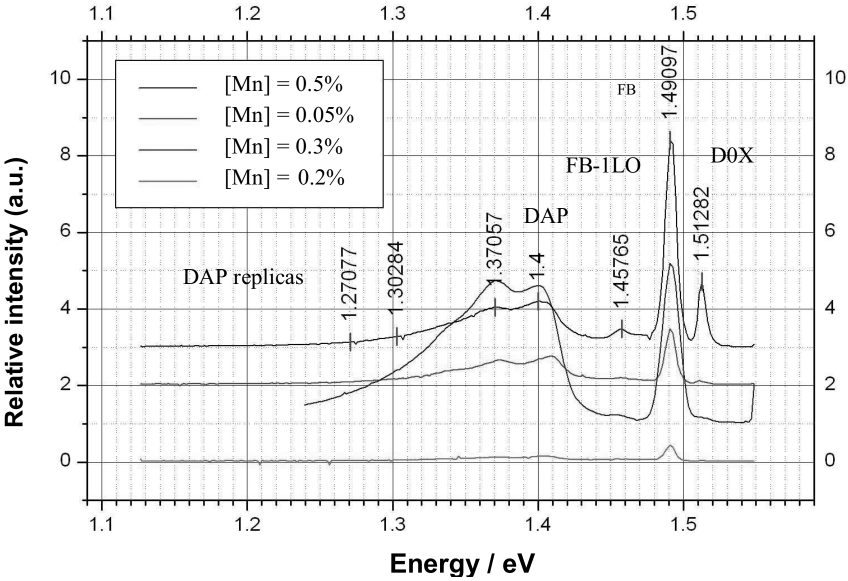

Fig 1. Photoluminescence spectra of (Ga,Mn)As samples grown by MOVPE.

2.4 Final Report: Electron Physics Group (EPG), Micro and Nanosciences Laboratory, Helsinki University of Technology (TKK)

The ferromagnetic semiconductor thin films of Mn-doped GaAs have been grown successfully by using molecular beam epitaxy. The ferromagnetism was observed through the resistivity and Hall-effect measurements. There is a peak in the resitivity at the Curie temperature (Fig.2.) as a result of the exchange interaction between the localized magnetic 3d electrons of Mn and the charge carriers in the valance band. The magnetization of the samples could be determined from the measurements of the anomalous Hall effect (Fig 3.), in which the Hall resisitivity depends on the external magnetic field in a non-linear manner due to the dependence of the effect on the magnetization. Therefore, by measuring the Hall-effect as a function of the temperature and the magnetic field one can determine the magnetization as a function of temperature. According to the experimental results the Curie temperatures of the (Ga,Mn)As samples have been estimated to vary within the range 40-75 K depending on the Mn concentration. This temperature can be increased by improving the fabrication technique. The Curie temperatures of the samples have been verified by using direct magnetization measurements in Belgium (Prof. Victor Moshchalkov's group, Katholieke Universiteit Leuven).

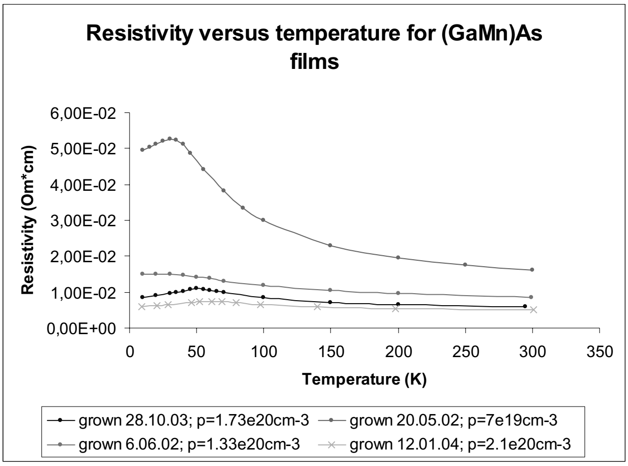

Fig. 2. Resistivity vs. temperature in (Ga,Mn)As at various temperatures.

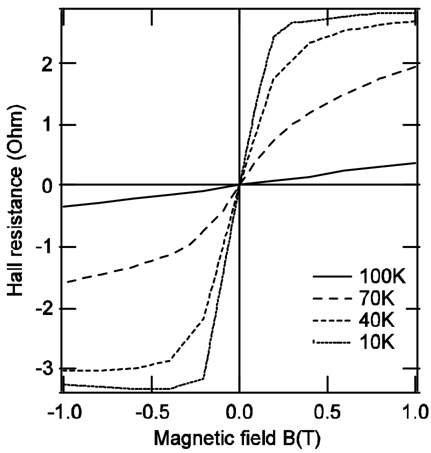

Fig.3. Hall resistance vs. magnetic field in (Ga,Mn)As at various temperatures. Mn composition is x=0.04.

We have fabricated the first ferromagnetic pn-junctions of Mn doped GaAs. In the samples, where also the n-side was heavily doped, we found a large magnetization dependent tunneling effect, for the first time. This phenomena can be used for the electrical spectroscopy of the valence band states, which complements the conventional optical techniques (Fig 4. - Fig. 6.).

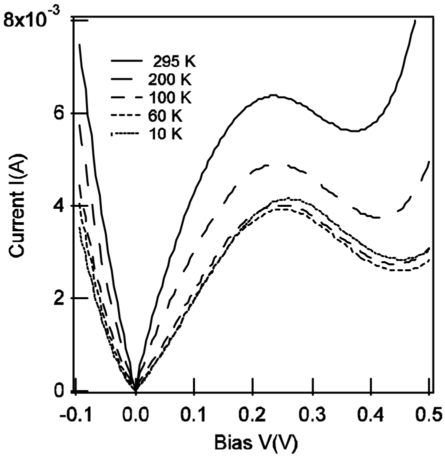

Fig.4. I-V characteristics of a ferromagnetic Zener diode at various temperatures ($B = 0T$).

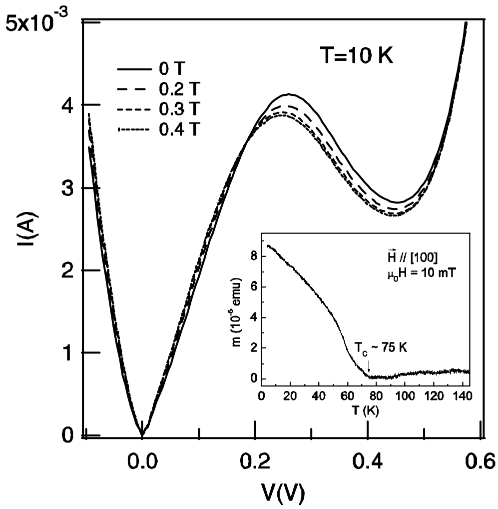

Fig.5. Measured I-V characteristics for a ferromagnetic Zener diode at T=10 K <T_C in various magnetic fields. The inset shows the magnetic moment m vs. temperature T in the (Ga,Mn)As/GaAs diode measured by using a vibrating sample magnetometer at $\mu_0 H = 10mT$, T_C is the Curie temperature.

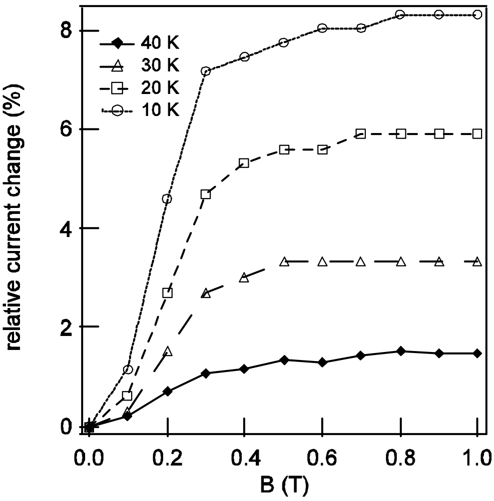

Fig. 6. Relative change of the tunneling current vs. magnetic field at V=350 mV and at various temperatures in a ferromagnetic Zener diode. The relative current change is defined as an absolute value of *(I(B)-I(0))/I(0).*

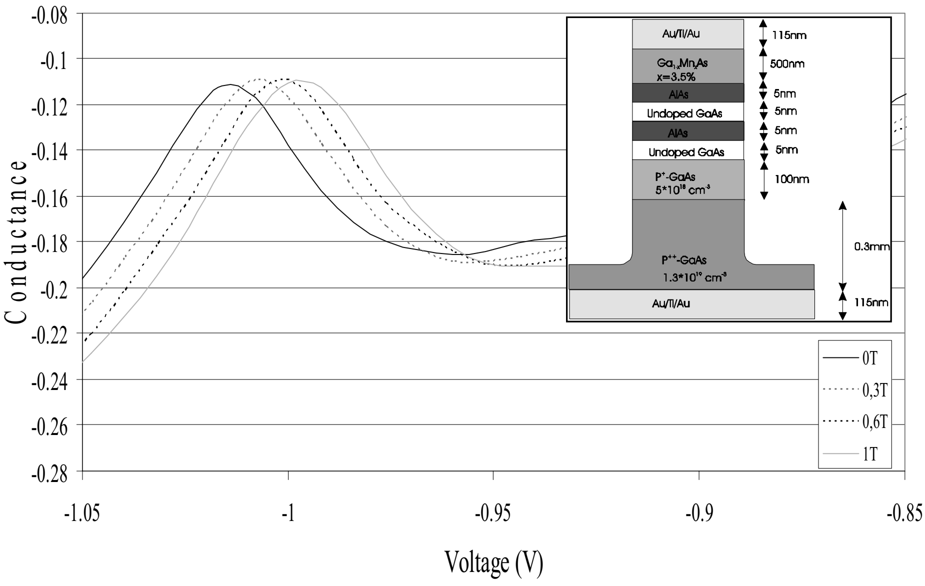

Fig. 7. Conductance as a function of bias voltage in various magnetic fields at 8 K in a magnetic resonant tunneling diode (RTD). The inset shows the schematic structure of the magnetic RTD.

We have also fabricated a ferromagnetic resonant tunneling diode based on the (Ga,Mn)As/AlAs –material system. The quantum well structure was grown in the Optoelectronics Group by using MOVPE and then the magnetic emitter was grown by using MBE. The measured I-V characteristics show the resonant tunneling peaks corresponding to the quantized heavy and light hole states in the quantum well. As a new effect a strong magnetic field dependence was observed in the resonance peaks at low temperatures (Fig. 7).

We have succeeded in the growth of the ferromagnetic (Ga,Mn)N thin films, as one of the first groups in Europe, by using the molecular beam epitaxy. In this method first a thin layer of Mn was grown on top of the GaN substrate, and then magnanese was diffused into the sample at elevated temperatures. The ferromagnetism of the samples was explored by using Hall effect measurements, magnetoresistance, and sheet resistance. To confirm the room temperature ferromagnetism in our samples, we have measured the magnetization as a function of temperature, which gave the Curie temperature of 330 K (Fig. 8.). The measured charge carrier concentrations in our n-type samples have been rather high, about 10^{20} cm^{-3} , and consequently the electron mobility has been only weakly temperature dependent. We also fabricated pn-junctions of Mn-doped GaN, where the magnetic side was of n-type. However, the I-V characteristics showed no exceptional magnetic field dependence.

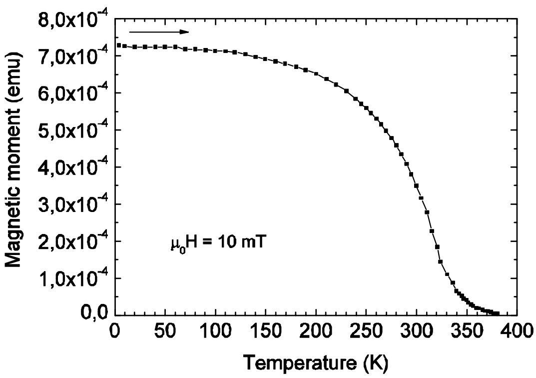

Fig. 8. Magnetization as a function of temperature in (Ga,Mn)N

In order to model the experimental results in Mn-doped GaN we have developed a mobility model, where we combine impurity scattering, optical phonon scattering, and spin-spin scattering. The model has been implemented in matlab, where the model can be fitted to the experimental data. In this way, e.g., the exchange interaction parameter for charge carriers has been determined for the first time, which is one of the most interesting new parameters in the ferromagnetic semiconductors.

2.5 Final Report: Positron Research Group, Laboratory of Physics (LP), Helsinki University of Technology (TKK)

One theme has been to study the point defects in magnetic semiconductors, and their role in the magnetic properties. The work of the positron group, TKK, in this theme started in GaMnAs alloys. We have used positron annihilation spectroscopy and infrared absorption measurements to study the Ga sublattice defects in epitaxial $Ga_{1-x}Mn_xAs$ with Mn content varying from 0% to 5%. The work then continued to the effects of Mn in wide bandgap semiconductors, namely GaN and ZnO, and in the latter Mn was revealed to have an important role in the reorganization of the crystal lattice during high temperature annealings.

Further, we have also initiated a study of Mn diffusion in GaAs, by combining radiotracer diffusion measurements and positron spectroscopy (in collaboration with Accelerator Laboratory, University of Helsinki). Both GaAs grown by MBE and LEC has been studied. The implantation of radioactive Mn took place in CERN in June 2005, and the annealing measurements during the following year. The results show that Mn diffuses mainly through two mechanisms, of which one (the slower one) is the migration of substitutional Mn by Ga vacancies. The faster diffusing component remains unidentified at this time.

Finally, in order to understand the role of manganese in the magnetic manganese-nitride alloys, positron experiments were performed also in the more simple binary systems, GaN and InN. We have extensively studied the doping of GaN, and identified vacancies, either in group-III or group-V sublattice, as the dominant point defects generated by doping with Si, O, or Mg. We have also investigated many different growth conditions and systems, ranging from bulk growth to different epitaxial methods. The influence on the lattice mismatch with substrate, and the interaction of vacancies and dislocations in general, have been extensively studied in GaN, and recently also in InN. We have expanded the studies also to cover the semiconductors closely related to nitrides and magnetic systems, namely ZnO and SiC.

2.5.1 Ga sublattice defects in (Ga,Mn)As

We have used positron annihilation spectroscopy and infrared absorption measurements to study the Ga sublattice defects in epitaxial (LT-MBE) $Ga_{1-x}Mn_xAs$ with Mn content varying from 0% to 5% (1×10^{21} cm^{-3}). Positrons annihilate as trapped at Ga vacancies in the layers, while the infrared absorption at 1.1 eV photon energy was used to determine the As antisite concentration [42]. We show (Fig. 9) that the Ga vacancy concentration decreases and As antisite concentration increases with increasing Mn content. This is in agreement with thermodynamical considerations for the electronic part of the formation energy of the Ga sublattice point defects. However, the absolute defect concentrations imply that they are determined rather by the growth kinetics than by the thermodynamical equilibrium. The As antisite concentrations in the samples are large enough to be important for compensation and magnetic properites. In addition, the Ga vacancies present at high concentrations are likely to be involved in the diffusion and clustering of Mn at low annealing temperatures. Our diffusion experiments (unpublished) and recent theoretical results [95] support this proposition.

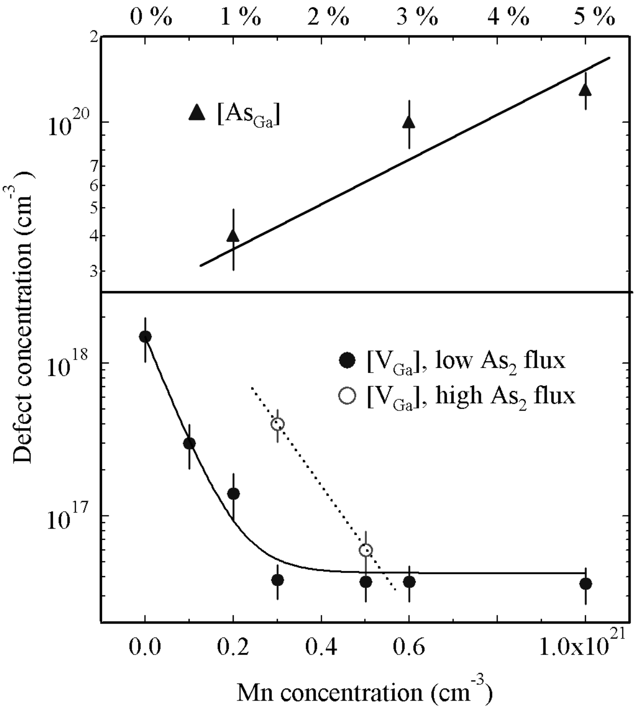

Fig. 9. The Ga vacancy and As antisite concentrations in the $Ga_{1-x}Mn_xAs$ layers as a function of the Mn concentration. The solid curve as well as the solid and dotted lines are drawn to guide the eye.

We have also investigated LT-MBE GaAs layers with less than 0.5 % Mn, namely in the range 0.02 – 0.3 % ($4 \times 10^{18} - 7 \times 10^{19}$ cm^{-3}). The positron results show that the Ga vacnacy remain constant when the Mn content is below 0.1 %, and starts decreasing with increasing Mn content above 0.1 %. This behavior is as expected from the thermodynamics, as the LT-MBE grown undoped GaAs is highly n-type (the electron concentration is in the $10^{19} - 10^{20}$ cm^{-3} range), and the Fermi level starts moving towards the valence band (increasing the formation energy of the Ga vacancies) only when the Mn content reaches similar values. On the other hand, the As antisite concentration increases slightly with increasing Mn content below 0.1 %, but decreases suddenly when the Mn content is further increased. As shown above, it increases again with increasing Mn content above 0.5 %. Hence it seems that around 0.1 - 0.5 % a reorganization of the fractions of different lattice sites of Mn occurs, leading to changes in the behavior of the compensating As antisite defects. Interestingly, a similar non-linear behavior of the lattice constant is observed at the same Mn concentrations [96].

2.5.2 Vacancy defects in (Zn,Mn)O

In our first studies on electron irradiated ZnO [31,48], we identified the Zn and O vacancies by combining measurements of the positron lifetime and Doppler broadening of the annihilation radiation to temperature-dependent Hall experiments, and by comparing the experimental observations with theoretical positron calculations. We then used this information to study the difference in the vacancy distribution between undoped bulk ZnO and $Zn_{0.985}Mn_{0.015}O$ crystals grown by chemical vapor transport [64]. They were grown at a temperature of 1100 °C in Zn-rich conditions, and subsequently annealed in O_2 (O-rich conditions) at 1000 °C. The positron lifetime experiments were performed at 10 − 500 K (see Fig. 10).

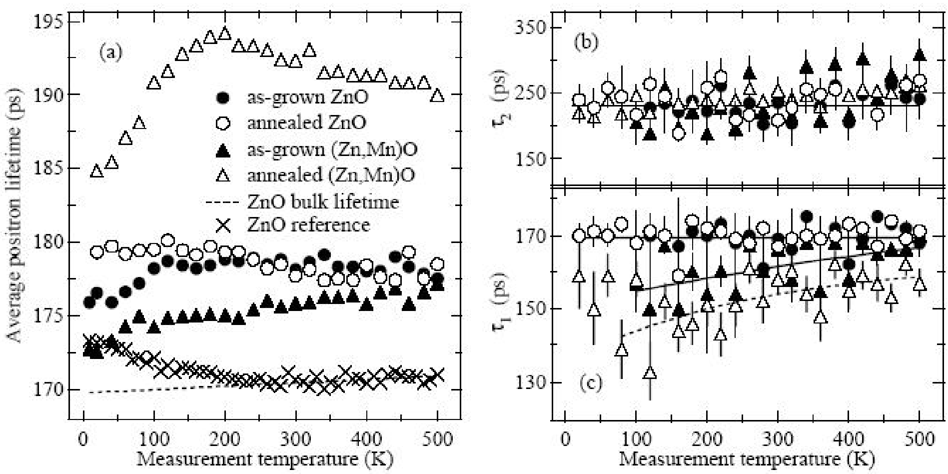

Fig. 10. The average positron lifetime (a) and the two separated lifetime components (b, c) as a function of measurement temperature in the (Zn,Mn)O samples. No positron trapping at vacancy defects is observed in the ZnO reference above 300 K, and the dashed line in (a) shows the fitted bulk lifetime, where the temperature dependence is due to the thermal expansion of the lattice. The lifetime value of about 230 ps in (b) is indicative of positrons trapping at Zn vacancies. The lower lifetime component (τ_1) is well below the bulk lifetime of 170 ps when the one-defect trapping model is valid (c). The lines in (b) and (c) are drawn to guide the eye.

The annealing in O_2 at 1000 °C has only a small effect (Fig. 1a) on the positron data in the ZnO sample, the most prominent being the decrease in the signal from negative ion type defects, i.e. the flattening the average positron lifetime (τ_{ave}) vs. temperature (T) behavior below 200 K. On the other hand, the positron lifetime in the $Zn_{0.985}Mn_{0.015}O$ sample changes significantly after the thermal treatment, due to a dramatic increase of the signal from the Zn vacancies. In addition, the clear increase of τ_{ave} with decreasing temperature above 200 K indicates that a significant part of the additional Zn vacancies are in the negative charge state. No evidence of vacancy clustering is observed due to the annealing of the samples, as the higher lifetime component (τ_2) is not affected by the thermal treatment (Fig. 1b).

The concentrations of the Zn vacancy related complexes in both as-grown and annealed ZnO samples can be estimated as $[V_{Zn}] = 2 \times 10^{16}$ cm^{-3}, and the concentration of the O vacancies can be estimated with trapping rate analysis as $[V_O] = 10^{17}$ cm^{-3}. The concentration of the negative ions in the as-grown ZnO sample is of the same order of magnitude as that of the Zn vacancies, and it decreases by an order of magnitude in the annealing. The concentration of the Zn vacancies in the as-grown $Zn_{0.985}Mn_{0.015}O$ sample is $[V_{Zn}] = 2 \times 10^{16}$ cm^{-3} as well, and the negative ion type defect concentration is similar. A significant part of the Zn vacancies is in the negative charge state after the annealing, and their concentration has become an order magnitude larger, $[V_{Zn}] = 2 \times 10^{17}$ cm^{-3}, while the concentration of the negative ions remains unchanged. No evidence of O vacancies is observed in the $Zn_{0.985}Mn_{0.015}O$ samples.

In summary, the high temperature annealing does not change the vacancy distribution in ZnO, while it increases the Zn vacancy concentration by an order of magnitude in $Zn_{0.985}Mn_{0.015}O$. Interestingly, the partial substitution of Zn by Mn in CVT-grown (Zn,Mn)O suppresses the formation of the O vacancies in Zn-rich conditions and enhances the formation of negative Zn vacancies in O-rich conditions.

2.6 Final Report: VTT Micro and Nanoelectronics (VTT)

VTT Micro and Nanoelectronics has reprocessed various sample geometries from a 100 nm thick Ga(Mn)As layers grown on semi-insulating GaAs (100) substrate by molecular beam epitaxy (MBE) at the Electron Physics Group (TKK). First an undoped GaAs buffer layer (230 nm) was grown at 580 ºC. Then low temperature MBE of a 100 nm thick $Mn_xGa_{1-x}As$ device layer was performed at 230 ºC.

In the experiments we studied samples with manganese concentrations of x=3.7 % and 4.0 % and Curie temperatures of 60 K and 62 K, respectively. The MnGaAs films were patterned utilizing UV-lithography and wet etching. Metal electrodes were fabricated by using either wet etching or lift-off process yet without seeing any process dependent difference in junction quality. Samples were electrically characterized down to 250 mK using He^3-sorption cryostat, standard electrical transport measurement set-up and lock-in techniques.

2.6.1 Material characterization at low temperatures

The material characterization was performed by measuring a temperature dependence of resistivity down to 280 mK temperature and by measuring a Hall resistance at 4.2 K and sub-Kelvin temperatures. The results of Hall measurement and the sample geometry are presented in Fig. 11. The temperature dependence of resistivity is shown in Fig. 12.

The Hall-resistivities ρ_{xy} (Fig 11.) exhibit the standard anomalous Hall effect: at low magnetic fields B (<0.4 T) ρ_{xy} shows a rapid increase with increasing B and then it almost saturates at B ~ 0.4 T. Additionally, ρ_{xy} (B) shows hysteretic behavior. The observed features in ρ_{xy} are well known signatures of ferromagnetism [1].

Figure 12 presents measured resistivity $\rho(T)_{xx}$ as a function of temperature. The resistivity of both samples show a peak around 60 K. The position of the peak gives the Curie temperature. The low-temperature resistivities were around $\rho^{x=3.7\%}(4.2K) \approx 6\ m\Omega \cdot cm$ and $\rho^{x=4.0\%}(4.2K) \approx 8\ m\Omega \cdot cm$, which are in good agreement with recently measured values at 4.2 K [89].

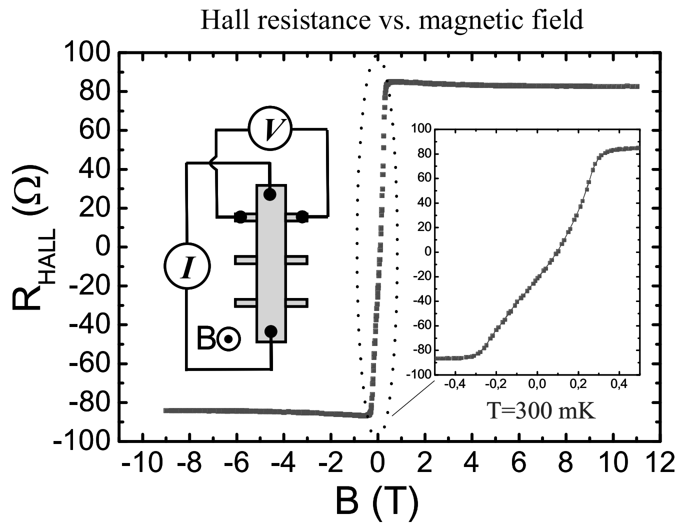

Fig. 11. Magnetic field dependence of Hall resistance and resistivity of $Mn_xGa_{1-x}As$ with x=3-7% manganese concentration. The field was applied perpendicular to the sample surface. The lower inset presents the geometry of the Hall measurement. The thickness of the MnGaAs layer was 100 nm.

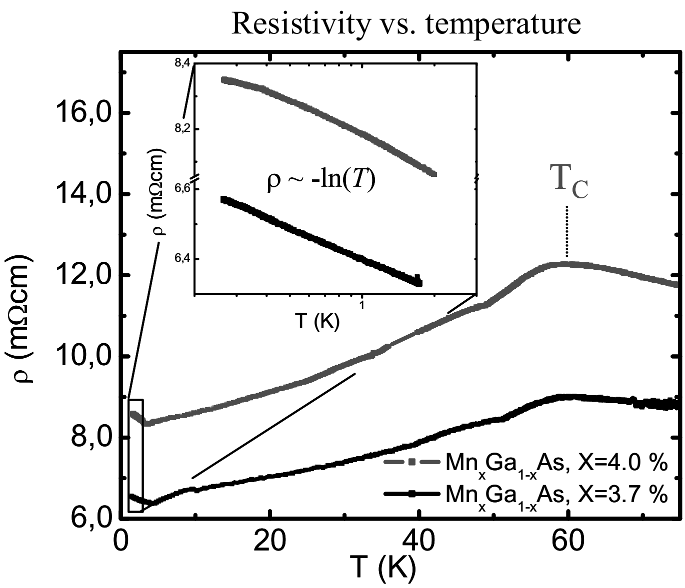

Fig. 12. Temperature dependency of the resistivity ρ. The inset presents a blow-up of the sub-Kelvin region results.

Below T ~ 5 K both samples exhibit a “Kondo-like” $\rho(T)\ \alpha\ \log(T)$ behavior (inset in Fig. 12) [2]. Such behaviour could be explained in terms of the Kondo effect arising from the presence of Mn interstitials in the $Mn_xGa_{1-x}As$ films [90].

2.6.2 Energy transport between hole-gas and crystal lattice:

We investigated a temperature dependent energy transfer rate between hole gas and lattice in thin $Mn_xGa_{1-x}As$ (x=3.7% and 4.0%) films by heating the hole system with power density P_d and measuring the hole and lattice temperatures T_h and T_{ph}.The $Mn_xGa_{1-x}As$ mesas were contacted with superconducting electrodes (Nb or Al) for preventing thermal leakage during the heating experiments. The well defined temperature dependency of the resistivity provides a local thermometer (inset in Fig. 12), which is utilized in the heating experiments: the resistivity of adjacent electronically isolated films gives the hole T_h and phonon temperatures T_{ph} in the spirit of Refs. [91,92] (see Fig. 13). The thermometers were first calibrated by slowly adjusting the bath temperature of the cryostat. Then one of the 5 μm wide adjacent $Mn_xGa_{1-x}As$ mesas was heated by applying a DC current density J at constant bath (cryostat) temperature. The change in the resistivities, which were measured with a small ac-signal, give the response of T_h and T_{ph} to heating power density $P_d = \rho J^2$. These responses are plotted in Fig. 10 at various bath temperatures.

The temperatures of electrically isolated phonon and hole thermometers have very different responses. The hole temperature shows a strong response while the phonon temperature shows only extremely weak increase, which is observable at the highest heating powers and lowest bath temperatures. This indicates that the thermal coupling between GaAs substrates and cryostat’s sample holder (copper) was extremely good, contradictory to studies utilizing silicon substrates [91,92]. Further, this also shows that the “bottle-neck” in the heat path is the hole-phonon energy relaxation rate.

Figure 14 shows also curves $P_d \propto T^n$ with n = 4,5. We can observe that the experimental T_h fall between these dependencies at high power density. More careful inspection reveals that the sample with x = 3.7 % (4.0 %) is described better with n=4 (n=5). On the other hand, the sensitivity of our hole (and phonon) thermometer is rather limited, which makes clear distinction between these two power laws difficult. Thus, we conclude that our preliminary experiments indicate that $P_d \propto T^n$ with n = 4 - 5 for both x = 3.7 % and x = 4.0 %. Note that as the hole-phonon energy relaxation rate is given by $\tau_{h-ph}^{-1} \propto T^{n-2}$ [93] our results also suggest that in $Mn_xGa_{1-x}As$ $\tau_{h-ph}^{-1} \propto T^{2-3}$.

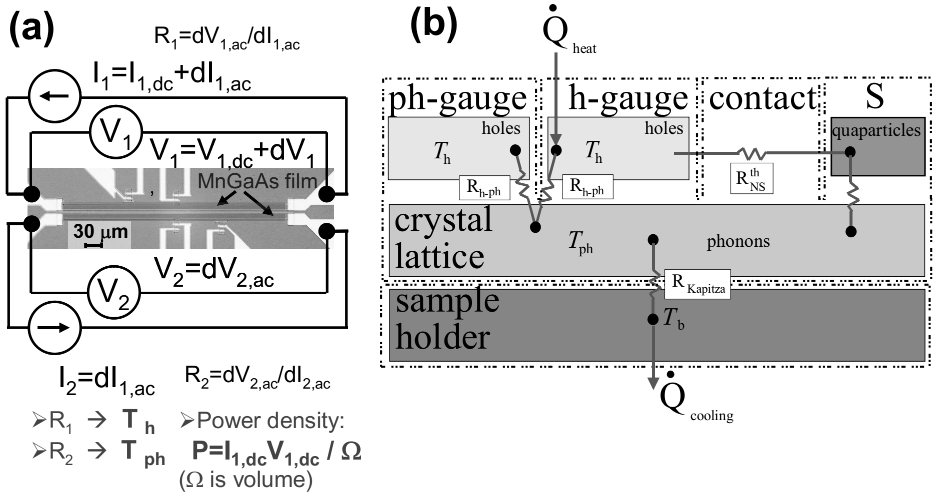

Fig. 13. A schema of energy transport measurement set-up . b) The simplified block diagram of the heat flow from heated structure (h-gauge) to the sample holder.

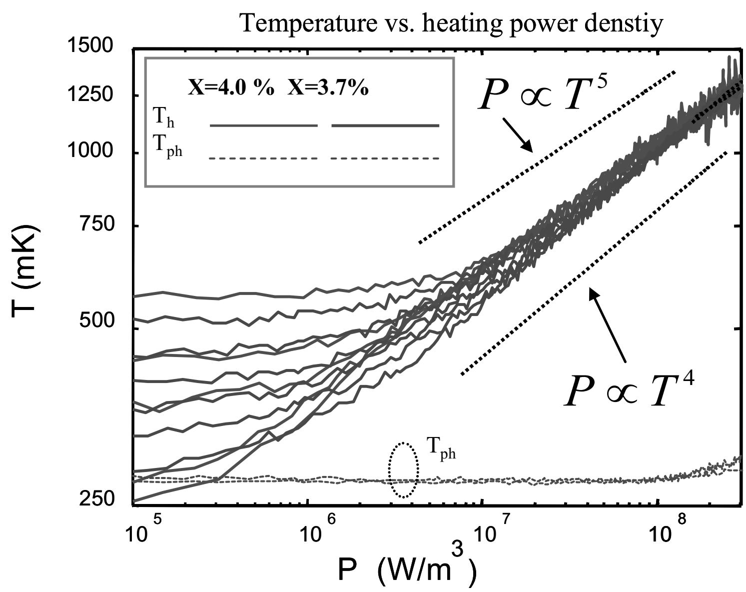

Fig. 14. Hole-gas temperature (T_h) and temperature of the lattice (T_{ph}) as a function of heating power density at various base temperatures..

The role of ferromagnetism in the energy relaxation is not yet clear. However, we have also performed heating measurements at various perpendicular magnetic fields between -

2 T and 2 T and our conclusion is that the hole-phonon relaxation rate in $Mn_xGa_{1-x}As$ has negligible magnetic field dependency.

2.6.3 Superconductor-ferromagnetic semiconductor junctions

We performed also a quantitative analysis of electrical junctions between different superconductors and $Mn_xGa_{1-x}As$ films by measuring resistances of aluminum and niobium contacts at various magnetic fields and at different temperatures. The measured contact resistances are small as compared to $Mn_xGa_{1-x}As$ sheet resistivity at the whole measured temperature range (at RT $R_j < 1\ \Omega \cdot \mu m^2$). Consequently, the linear current voltage characteristics measured at 4.2 K in addition to the small junction resistances indicate that high quality Ohmic contacts were formed between aluminum or niobium contacts and the $Mn_xGa_{1-x}As$ film.

Figure 15 present a normalised conductance of Al/ $Mn_xGa_{1-x}As$ and Nb/ $Mn_xGa_{1-x}As$ contacts as a function of bias-voltage at 280 mK temperature and at various magnetic fields. At sub-Kelvin temperatures both Al/$Mn_xGa_{1-x}As$ and Nb/$Mn_xGa_{1-x}As$ junctions exhibit strongly non-linear *IV*-characteristic (see Figs. 15 and 16). With larger voltages junctions have linear *IV*-dependence, but at zero-bias regime conductances are reduced.

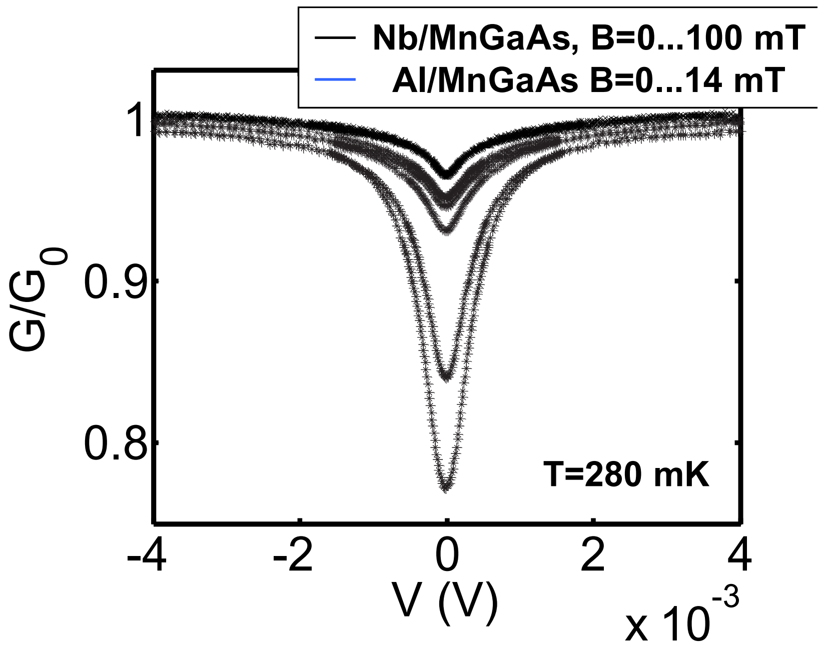

Fig. 15. Normalized conductance of the Al/ $Mn_xGa_{1-x}As$ and Nb/ $Mn_xGa_{1-x}As$ junctions at various magnetic fields. The manganese concentrion x=3.7 %.

The zero-bias conductance of Al/$Mn_xGa_{1-x}As$ contacts introduces strong magnetic field dependence in contrast to Nb/$Mn_xGa_{1-x}As$ junctions, which are magnetic field independent in the measured magnetic field range ±1 T. This indicates that superconductivity plays a minor role in niobium contacts. One possible explanation is that the ferromagnetism of $Mn_xGa_{1-x}As$ destroys the superconductivity of niobium in the vicinity of Nb/ $Mn_xGa_{1-x}As$ junction. On the other hand, the magnetic field dependence of Al/$Mn_xGa_{1-x}As$ junctions saturates at magnetic fields larger than ~10 mT, which is in good agreement with the critical field of superconducting bulk aluminum (~10.4 mT). Thus, this is a clear indication that the superconductivity plays a role in Al/$Mn_xGa_{1-x}As$ junctions indeed.

The zero-bias conductance of ferromagnet/superconductor junctions are reduced due to the fact that the Andreev reflection probability at the interface is limited by the carrier density of the *minority* spin band at the Fermi level. This is schematically presented in Fig. 16 a). We used a model where the total current is divided into two independent parts: one describes conventional unpolarized system and another is a fully spin-polarized current with zero Andreev reflection probability. The total current may thus be written as

$$I_{total}(V) = I_{unpolazired}(V)\cdot(1-P) + I_{polazired}(V)\cdot P, \qquad (1)$$

where *P* is spin polarization. Different current contributions are calculated by using the model given by Mazin *et al.* [94]. The used model describes a diffusive system, where a contact area is much larger than a charge carrier mean free path.

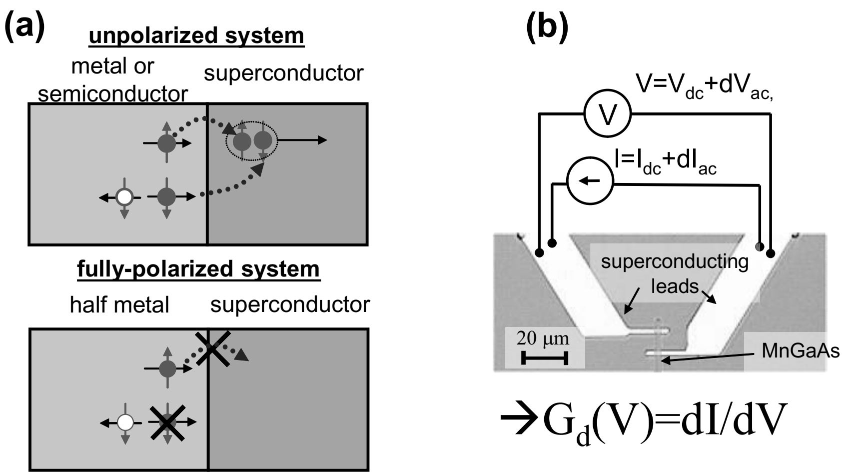

Fig. 16. a) A scheme of spin-polarisation reduced Andreev reflection. b) A schematical drawing of conductance measurement set-up. A bias-voltage is applied across a whole $R_{total}=2xR_{junction}+R_{mesa}$ system.

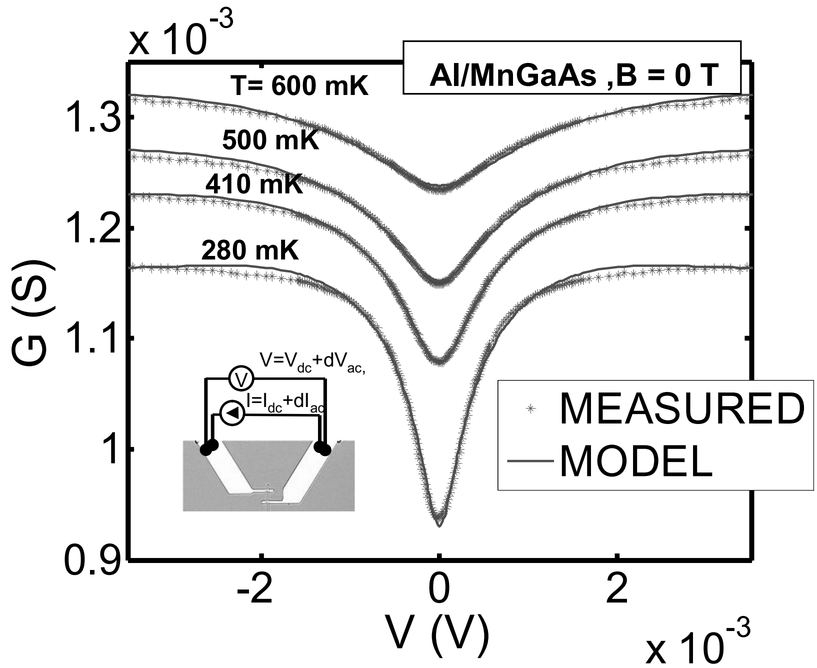

Fig. 17. The conductance of the Al/ $Mn_xGa_{1-x}As$ junctions at different temperatures between 280 mK and 600 mK. A solid red lines are a fit of a used model. The results at different temperature are shifted for clarity.

We performed conductance measurements of Al/$Mn_xGa_{1-x}As$ junctions at various temperatures and the results are presented in Fig. 17. The solid lines are the best fits of the model described above to the data. Fitted polarisation *P* in MnGaAs is approximately 80 %, but due to large number of unknown fitting parameters of the used model the inaccuracy is large. However, the spin polarization of the $Mn_xGa_{1-x}As$ film clearly reduces current at low bias voltage regime and thus diluted ferromagnetic semiconductor-superconductor junctions may be used in suitable applications, namely, e.g., in microcoolers.

3 International Aspects

OEG is collaborating with Ioffe Physico-Technical Institute, St. Petersburg, Russia, in the development of GaN-based technology. OEG is also collaborating with Thomas Swan Ltd. and Epichem Ltd. in the development of MOVPE technology.

The Electron Physics Group has had a close collaboration with Prof. Victor Moshchalkov's group, Katholieke Universiteit Leuven, in magnetization measurements of Mn-doped GaAs and GaN. This collaboration has resulted in 4 joint publications.

In the present project the researchers of the Positron Research Group, TKK, have had direct international collaboration with 25 institutions. The researchers of the group have given 20 invited presentations in international conferences in 2003 – 2006. The Group has participated in one EU project (CADRES) and one NORFA project (NOCDAD) which are methologically (defect analysis) directly related to the present project. The Group is currently actively participating in the planning of four EU/FP7 projects (silicon technology, nitride optoelectronics, ZnO optoelectronics and magnetism in semiconductors). The Positron Group organized two international summer schools in the NORFA project in 2003 - 2004. Prof. Saarinen (subproject leader until the end of 2005) has been a member of four international advisory committees.

4 Publications and Academic Degrees

Table 2. Publications and academic degrees produced in the project. Numbers of different types of publications are given along with the reference numbers. List of refereed journal articles are given in Section 6.1, refereed conference papers in Section 6.2, monographs in Section 6.3 and theses in Section 6.4.

Partner	Type of publication	2003	2004	2005	2006	**Total**	Publication numbers
TKK, VTT	Ref. journal art.	8	10	13	24	**55**	1-55
	Ref. conf. papers	4	6	3	8	**21**	56-76
	Monographs	-	-	-	-	**0**	
	Doctoral dissert.	-	-	2	7	**9**	77-85
	Licentiate degrees	-	-	1	-	**1**	86
	Master degrees	1	-	1	-	**2**	87-88

5 Other Activities

The group leaders in the consortium have participated in informal meetings at least twice a year to discuss results and steer activities. Articles about the project have appeared both in the international press (Compound Semiconductors magazine) and in the domestic press (Prosessori and Kemia magazines).

6 Publications

6.1 Refereed Journal Articles

[1] J. Toivonen, T. Hakkarainen, M. Sopanen, H. Lipsanen, J. Oila and K. Saarinen, Observation of defect complexes containing Ga vacancies in GaAsN, Applied Physics Letters 82, 40 (2003).

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6.2 Refereed Conference Papers

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STRUCTURAL AND ELECTRICAL PROPERTIES OF SELF-ORGANIZING MOLECULAR MATERIALS (SOMOMA)

Ilkka Tittonen[1], Harri Lipsanen[2], Paavo Kinnunen[3], Adrian Sutton[4] and Kimmo Kaski[4].

Abstract

Cytochrome c (a membrane protein) participates in electron transfer chain in mitochondria, the structures contain ion channels and act as the ion exchange walls between organic cells. It has been found that complexes of cytochrome c and lipids arrange themselves into the large scale structures. One of the first discoveries of this self-organization effect was found by the group of prof Paavo Kinnunen at Biomedicum for cytochrome C. Similar type of process is strongly believed to be the cause of e. g. Alzheimer disease. Cytochrome C contains a heme group that can even be modified and in the center of this group iron is either Fe2+ or Fe3+. Formed unique fiber-like structures are interesting in medicine as self-organized structures and because of potentially interesting optical and electrical properties.

The liposomes are created by a self-assembly process of phospholipid molecules in an aqueous solution. The liposome comprises a phosphlipid bilayer vesicle and is closely related to a cell membrane. We have found that the liposomes themselves undergo a self-assembly process in the presence of cytochrome c forming bundles of threads in rope-like polymerized structures. We have also found that some of these structures are magnetic and some are not. Some of the ropes are twisted and the colouring varies between white and red. It is possible that other stable structures may be created by varying the concentrations of the liposomes and cytochrome c in solution and the temperature. The pH also influences the resultant structures.

However, the found process was not unique, but is a more general phenomenon, since similar type of self-organization has recently been found for a number of systems such as histone H1, cytochrome C, indolicinin, endostatin. Even for cytochrome C the outcome varies depending on the starting composition and also in the exact same process and even inside the same fiber (from amyloid to native). Mainly because of huge medical interest, the research activity concerning these self-organization effects has enormously expanded worldwide during this research project and a lot new data is now available.

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1 Partners and Funding

Helsinki Biophysics & Biomembrane Group (HBBG), University of Helsinki

HBBG is supervised by professor Paavo Kinnunen and the group now consists of 6 full-time postdoctoral fellows, 5 full-time graduate students, and one technician. To this project contributed Drs. Arimatti Jutila, Hongxia Zhao, Rohit Sood, Yegor Domanov, and Juha-Matti Alakoskela, as well as graduate students Tuula Nurminen, Christian Code, and Jussi Pirneskoski.

Micro and Nanosciences Laboratory, Micro and Quantum Systems Group, Helsinki University of Technology

MQS group is supervised by professor Ilkka Tittonen, the whole group consists of 8 graduate students of which to this project contributed MSc Päivi Sievilä, MSc Nikolai Chekurov and MSc Ossi Hahtela.

Optoelectronics Laboratory (OEL), Helsinki University of Technology (presently Micro and Nanosciences Laboratory)

The research group consists of subproject leader professor Harri Lipsanen and graduate student Hannu Koskenvaara.

Laboratory of Computational Engineering (LCE), Helsinki University of Technology

The research group consists of professor Kimmo Kaski, professor Adrian Sutton (also at Material Science at Oxford University, later Imperial College), and graduate students Sebastian von Alfthan, Jussi Kumpula and Kim Pihlström.

1.3 Funding

Table 1. Funding of the project in 1000 EUR in 2003-2006. Internal funding consists of manpower costs and operational expenditures provided by the organisation. The funding provided by the Academy of Finland and other external sources is also shown in the table.

Partner	Funding organisation	2003	2004	2005	2006	**Total**
OEL/HUT	Academy	12	24	23	13	**72**
	HUT	9	12	12	9	**42**
	Industry	0	0	0	0	**0**
LCE/HUT	Academy	16	32	31	13	**92**
	HUT	9	12	12	9	**42**
	Industry	0	0	0	0	**0**

MQS/HUT	Academy	15	31	30	13	**89**
	HUT	3	6	6	3	**18**
	Industry	0	0	0	0	**0**
HBBG/UH	Academy	18	38	39	19	**114**
	UH	9	12	12	9	**42**
	Industry	0	0	0	0	**0**

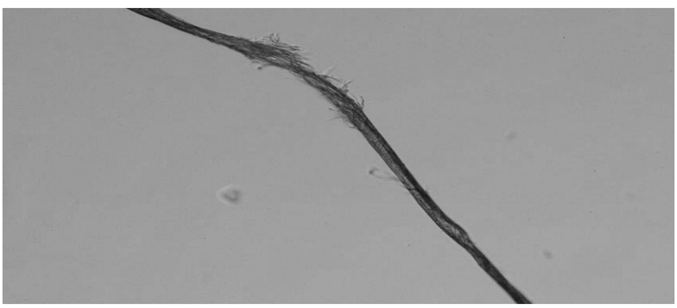
2 Research Work

2.1 Objectives and Work Plan

Objective of the project was to study organic fiber-like structures, various optical and electrical phenomena, various organic coatings and combination of organic structures with semiconductor micro/ nanosystems. Since the scale of self-organization was known to be extremely high, a lot of effort was to be invested in understanding the formation of these very large structures from orders of magnitude smaller building blocks. In addition, a lot of work was to be performed for combining various organic/semiconductor microsystems and studies of micromechanics.

2.2 Final Report: Common Themes and Collaboration

The basis to the project was the finding that cytochrome c, a well-established protein component (with a net positive charge) of the biological electron transfer chain in mitochondria, formed in the presence of proper negatively charged lipids fibrillar structures [1]. These fibers can be very long, up to one millimetre and their diameters vary between 10 to 20 microns. Optical microscopy is enough to reveal them to consist of smaller ‘subfibers’. Attempts to resolve their cross-sectional structure were futile. More specifically, when fibers were embedded in epoxy for cutting in a microtome, the blade just pulled the fibrils out of epoxy. The fibrils seem to be extremely durable against mechanical forces. Further studies under microscope showed them to be highly flexible.



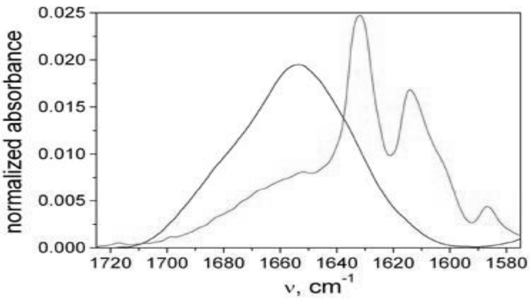
It was assumed that the redox properties of cytochrome c would be retained by these fibers and, accordingly, the fibers would conduct electrons. This, however, turned out not to be the case, as established in the experiments performed at HUT. The lack of conductivity is likely to be due because of the structural diversity of the fibers (see below). In spite of the above negative finding it was evident that it would be possible to control the organization of biomolecules by charged surfaces. Critical to this process is the electrostatically triggered nucleation of the cationic peptide/protein on the anionic liquid crystal surface. The latter was studied jointly with LCE (Kimmo Kaski and Adrian Sutton).

The modelling and simulation activity of the project was the responsibility of Laboratory of Computational Engineering (LCE) at Helsinki University of Technology (TKK) with professors Kimmo Kaski (LCE/TKK) and Adrian Sutton (LCE/TKK&Material Science/Oxford and later Physics/Imperial College) acting jointly as subproject leaders and student supervisors. The modelling and simulation subproject was planned to be closely related to experimental work done in the project. All the focus areas served the purpose of this project and the nanoelectronics programme acted importantly as good means of researcher training.

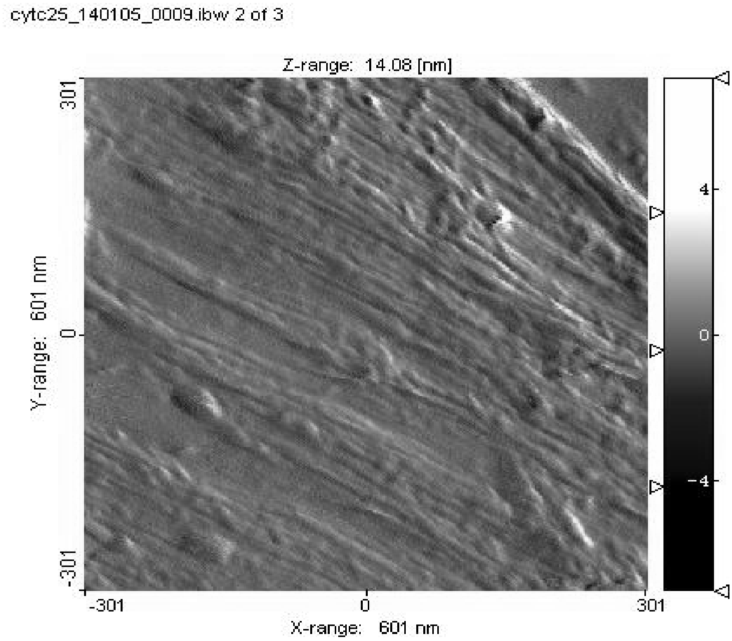
2.3 Final Report

Formation of fibrils

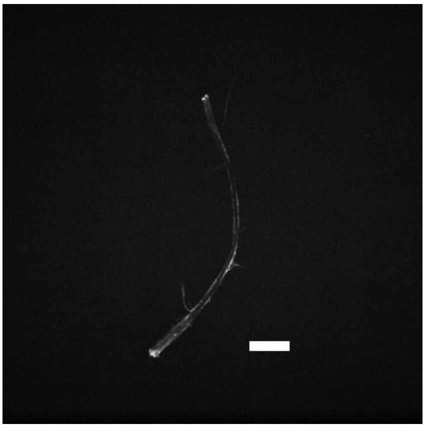
Following the initial finding of cytochrome fibril formation in the presence of acidic biological liquid crystalline amphiphiles, phospholipids [1] it was of interest to establish if this was a generic property of proteins. This was not the case but fibrils could only be made of proteins interacting electrostatically with the negatively charged amphiphiles because of carrying strongly cationic clusters as their surface structure [2]. Following the early characterization of the fibers by microscopy we proceeded into studying their more detailed structure. This was performed by Fourier transform infrared microscopy [3].

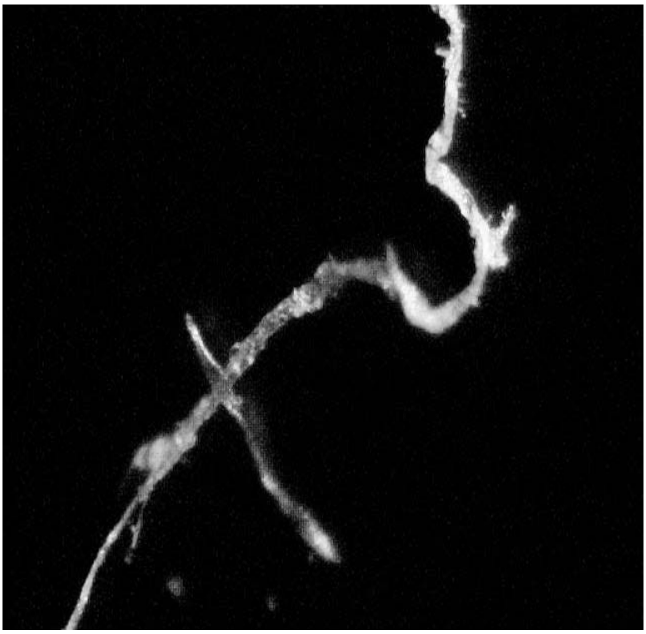


The most dramatic finding was that the conformation of the protein varies considerably even within a single fiber, demonstrating native structure (black line) and amyloid beta-sheet structure (red line) in the FTIR spectra. The latter structure readily comply with the exceptional mechanical properties of fibrils. The substructure of the fibrils was assessed from the surface by AFM, which demonstrated protofibrils of a diameter of approx. 3-4 nm (see below).

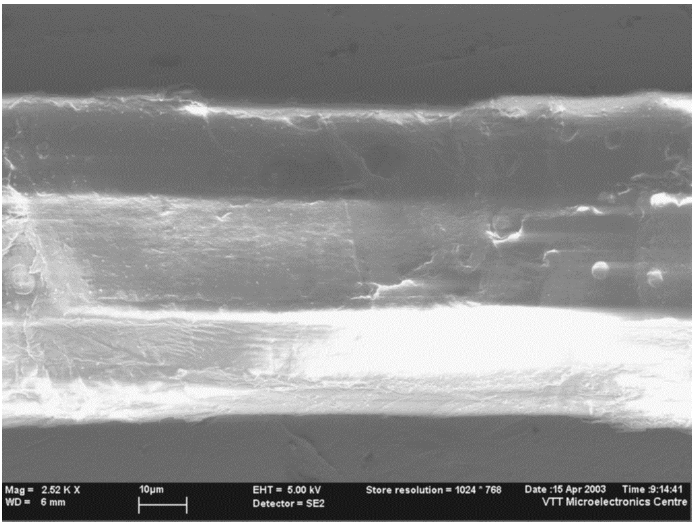


These fibrils could also be made of very simple and small synthetic peptides [2]. This is of major importance from the point of view of possible applications as these materials can be designed to molecular detail and are easily made synthetically. Because of the well-established chemistry involved, it is now possible to link different electronically/optically relevant moieties to these peptides prior to the fibril formation. The latter will then organize the said electronically/optically interesting groups into highly anisotropic fibrils in a controlled manner. An example of this is depicted below, showing protein labelled with a fluorescent group. Interestingly, fluorescence is only seen emanating from the fibril surface and the fibril ends, in essence demonstrating the fibril to act as an optical waveguide.

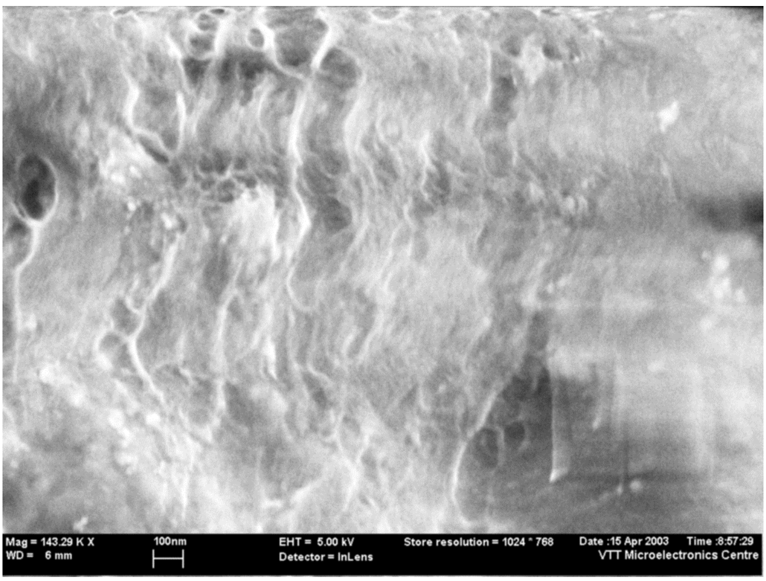




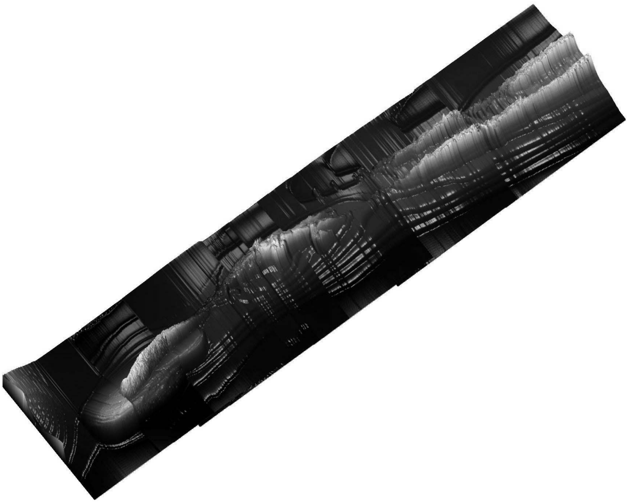
This image of the optical microscope (full scale is appr. 1 mm) reveals some properties of cytochrome c based fibrils. Individual structures vary a lot in shape and in colour. The red colour is believed to be due to the heme group. The red coloured fibril also shows typical twisting of the structure.



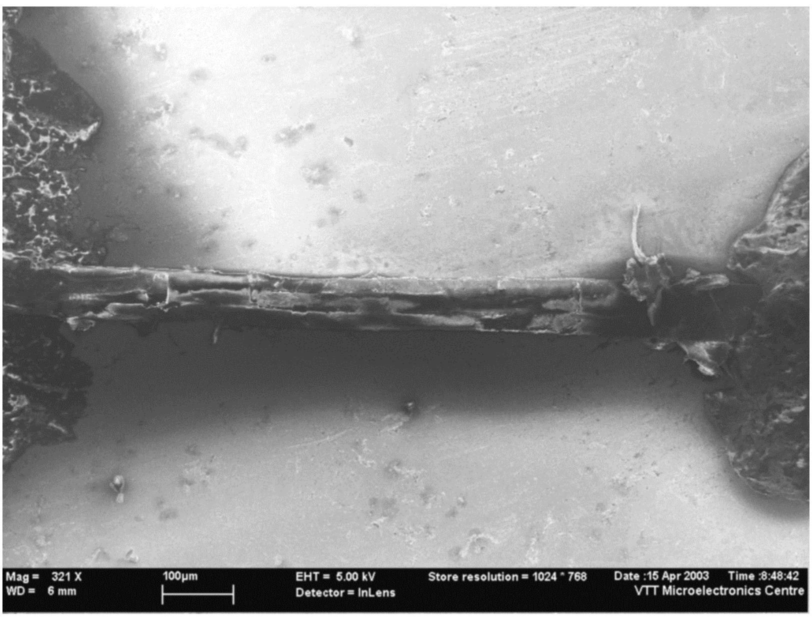
SEM-images (courtesy of J. Ahopelto at Micronova/VTT) give a bit better understanding of the macroscopic formation of the fibres. One can see, that one fiber actually consists of three individual structures that have become ‘glued’ together. The surfaces are relatively smooth with rather weak crater like shaping. A thorough understanding of the whole self-organization process would require in situ microscopic imaging which could not be established during this project but will be pursued in the future. Since the creation of these structures is also of enormous importance in medicine, this planned research will be worth the effort.



This SEM image shows 100 nm size inclusions on therwise rather smooth surface.



This reconstructed AFM study of one fiber shows the twisting and crossing of the structures in more detail.

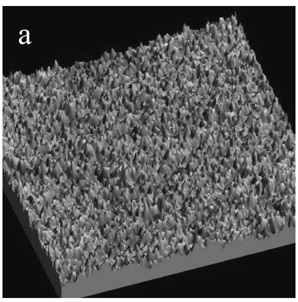


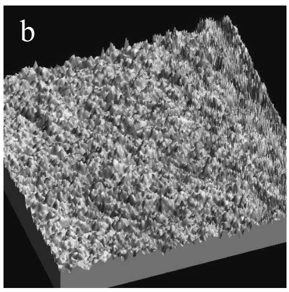
In electrical measurements a major difficulty was encountered in creating good contacts since the adhesion and atomic level structures of these almost macro objects were not known. Various ways to establish a contact was tried. A number of indium based soft metal contacts were tried but no macroscopic electrical conductivity was found. In the macroscopic scale, the resistivity higher than $10^{10}\Omega$/mm was measured. This could however be lowered a bit by iodine treatment of the fiber surfaces. One reason for this might be in the self-organization process even though the original structures participate in the ion channel dynamics between organic cells.

One of the biggest discoveries of this project was the finding of magnetic ordering [5]. This effect was highly unexpected and to our knowledge has not ever been observed before for this kind of organic systems. The experiment was very easy, in aqueous solution, some of the fibers were served to move towards a permanent magnet whose strength was approximately 10 mT. This observation could easily lead to a simple practical method to collect, separate and move fibers in a liquid. A drawback or a pecualiry is that only some fibers responded to the gradient of the magnetic field. This effect is not fully understood but a good guess would be to relate this effect to the hem groups that contain iron and as a result of the self-organization process various hem groups can be transferred very close to each other showing magnetic ordering in some of the fibers.

Organic functionalisation of InGaAs/GaAs surface quantum wells

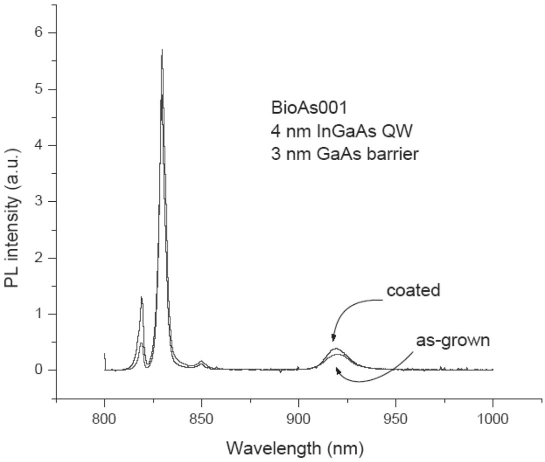
Functional combination of organic molecules and nanostructured semiconductors has potentially interesting sensor applications, such as highly sensitive detection of adsorbed molecules on a surface. GaAs-based nanostructures, especially near-surface quantum wells and quantum dots are promising candidates for this due to their high structural and electronic quality. In our experiments self-assembled monolayer of octadecylthiol (ODT) is used for the stabilization of the GaAs surface. The ODT-coating process produces smooth surfaces with rms roughness of 0.56 nm (vs. 0.33 nm in a reference GaAs surface) as shown in the AFM images.





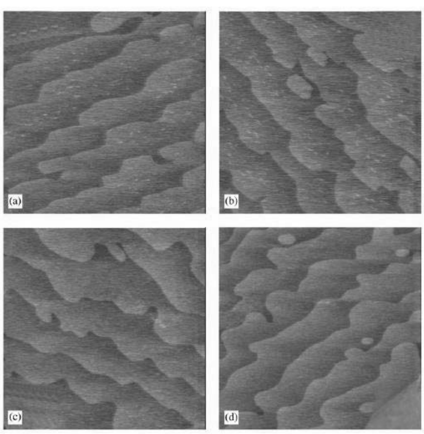
A reference (a) and ODT-coated (b) GaAs (100) surface imaged by atomic force microscopy.

Near-surface InGaAs/GaAs quantum well structures were grown by metalorganic vapor-phase epitaxy [6]. The sample consists of a 4 nm $In_{0.20}Ga_{0.80}As$ quantum well separated by either a 3 or 6 nm GaAs barrier from the surface. Stabilization of the ODT-coated GaAs surface was probed by low-temperature photoluminescence measurements shown in the figure above. The ODT-monolayer results in slight increase in the QW luminescence at 940 nm. The strong peaks at around 820 –830 nm originate from GaAs. This is promising because any surface modification typically destroys the luminescence signal unless special surface passivation procedures are used. We have developed a novel surface passivation technique that utilizes a few monolayers thick epitaxial GaN layer on the surface [7]. By combining this to the ODT-monolayer we expect several orders of magnitude higher sensitivity to the surface adsorption. The results from the organic surface modification are reported in Ref. [8].

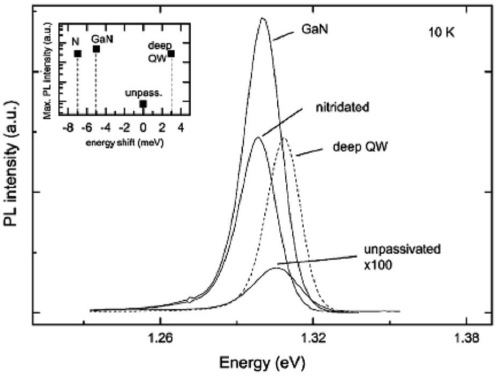


Photoluminescence (T = 10 K) spectrum of ODT-coated near-surface quantum well as compared to as-grown reference sample. The quantum well luminescence is seen at the wavelength of 940 nm.

An attractive passivation material for biological applications of semiconductor surfaces is gallium nitride (GaN). Ultrathin GaN passivation layers were grown in situ on near-surface InGaAs/GaAs quantum wells using metalorganic vapour-phase epitaxy (MOVPE) with dimethylhydrazine as nitrogen source [7]. Nitridation of GaAs using DMHy during the post-growth cool-down to form thin GaN layer was also studied. The effect of passivation on the surface recombination rate of quantum well structures was characterized using low-temperature (10 K) photoluminescence. The GaN surface has very hard diamond-like structure and the morphology is smooth and ordered in atomic scale as shown in the figure below. Measured after growth, the GaN passivation was shown to enhance the PL intensity of the near-surface QWs approximately by a factor of 20. For samples stored in ambient air for 5 months, the enhancement is nearly 10^3. The results suggest that MOVPE-grown thin GaN layers are applicable to GaAs surface passivation. Another semiconductor nitride, InN, is interesting in applications where a longer wavelength (>1.5 μm) is desired. However, the quality of the material is still quite far from that required for practical applications [10].

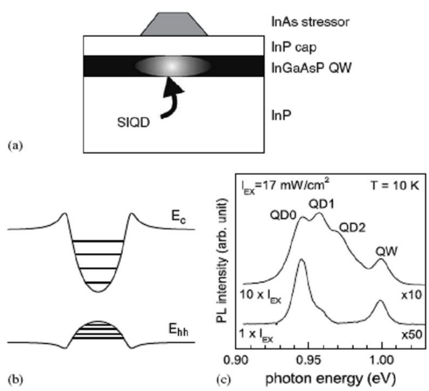


AFM micrographs of (a) deep-QW, (b) unpassivated, (c) GaN-passivated, and (d) nitridation-passivated near-surface QW samples. No clear difference can be observed between (c) the epitaxial GaN layer and (d) the nitridated GaAs surface. The scan size is 3x3 μm^2 and the vertical scale is 3 nm. Atomic steps are clearly visible in all samples.

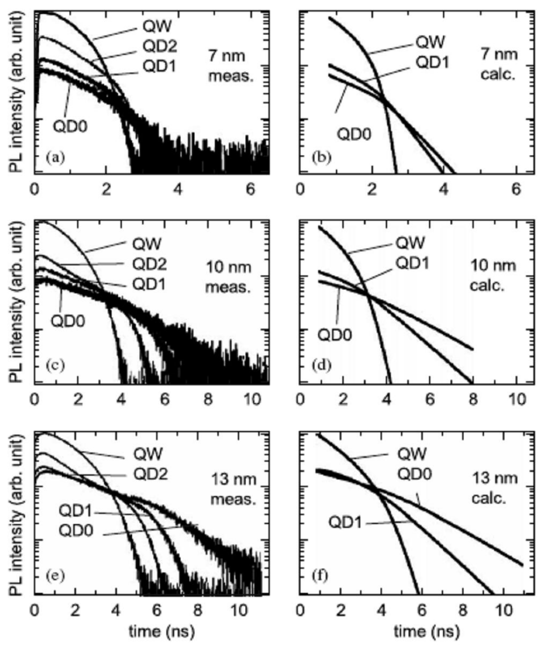


PL spectra of passivated 4 nm thick $In_{0.25}Ga_{0.75}As/GaAs$ near-surface QWs after samples stored about 5 months in ambient air. The intensity of GaN-passivated sample is nearly three orders of magnitude larger compared with unpassivated sample.

In addition to two-dimensional QW structures, various zero-dimensional quantum dot (QD) structures were fabricated and studied. Coherent Stranski–Krastanow growth is known to be applicable in the fabrication of semiconductor quantum structures. One way to utilize self-assembled islands in the fabrication of quantum dots (QDs) is to use these islands as stressors [23]. The tensile strain underneath the islands reduces locally the band gap of a near-surface quantum well (QW). The resulting lateral confinement potential is nearly parabolic for both electrons and holes, and the vertical confinement is achieved by the interfaces of the QW. The important advantage of the strain-induced quantum dot (SIQD) approach is the possibility to optically measure and straightforwardly model the strain effects caused by the self-assembled islands. What is more interesting, the SIQDs provide a viable means to study the carrier dynamics in nearly perfect zero-dimensional systems as well as the interaction of the QW and the islands on the surface.
Carrier dynamics of novel strain-induced InGaAsP/InP quantum dots (QDs) were investigated in Refs. 9, 11-12. In this structure, self-assembled InAs islands on the surface act as stressors and create a lateral confinement potential in the near surface InGaAsP/InP quantum well. PL measurements reveal that decreasing the distance from the QD to the surface significantly diminishes the QD–PL intensity, presumably due to surface states of the InAs islands. Moreover, time-resolved photoluminescence (TRPL) measurements showed a faster decay of the QD–PL with decreasing distance. To analyze the carrier dynamics, rate equation model is applied and surface state-related transitions were taken into account. The model is found to agree with measurements, and thus provides a possible explanation for the observed temporal behaviour of the carriers.



(a) Structure of the SIQD sample. (b) The schematic deformation of the conduction band and the heavy hole band in the InGaAsP QW. Discrete energy levels of the induced QD are also shown. (c) PL spectra from SIQD sample measured with different excitation intensities. Positions of the QW and three quantum dot (QD0–QD2) peaks are marked in the picture.



TRPL results from the samples with a cap layer thickness of (a) 7 nm, (c) 10 nm, and (e) 13 nm. PL intensity curves from the QW, QD0, QD1, and QD2 states are shown. The corresponding rate equation calculations to TRPL results are shown in (b), (d), and (f).

Precipitation of NaCl crystals on lipid monolayer

The project centred on simulations of experiments by Professor P Kinnunen's group at Biomedicum in which precipitation of NaCl crystals from an *under*saturated aqueous saline solution was observed to be catalysed by a lipid monolayer. An open source molecular dynamics program GROMACS was used to carry out these simulations. In the experiments by Kinnunen's group the dipalmitoylphosphatidylcholine (DPPC) layer is dicationic, i.e. there are ions present at the surface with positive electronic charges. It was also considered significant that the spacing between the lipids in the experimental monolayer is commensurate with the lattice parameter of the NaCl crystal lattice.

Initially we made attempts to use a DPPC lipid model in the simulations to see whether NaCl crystals could be grown from the saline solution. However, these attempts failed and it was thought that a principal reason for the failure was that the spacing of the lipid molecules was *in*commensurate with the NaCl crystal lattice. In principle this failure of the model could have been rectified by fine-tuning the parameters of the force-field describing the lipid, but this would have taken far too long for a summer project. In addition the dicationic nature of the real lipid surface was not reproduced by the DPPC model. For these reasons we decided to simulate the dicationic environment presented by Kinnunen's DPPC layer with a (100) layer of Na^+ ions and a parallel (100) layer of Cl^- ions immersed in aqueous NaCl solutions. The spacing on the ions in the ionic layers was the same as those in a (100) surface of NaCl. Although this is a considerable simplification of the real experiment it had the virtue of enabling us to test our intuition that the surface of the lipid acted a catalyst for the precipitation of NaCl crystals by providing a favourable ionic environment for these crystals to grow from the aqueous solution. In effect we envisaged the lipid as providing a site for heterogeneous nucleation of NaCl crystals from solution. If this intuition were correct we should see Na^+ and Cl^- ions coming out of aqueous solution and attaching themselves to the ion layers.

The very early stages of such a precipitation reaction were seen in the simulations. However, exceedingly long run times and somewhat unrealistically large saline concentrations (ten times those of the experiments) were needed to see any significant crystal growth. This reflects the sluggish dynamics of Na^+ and Cl^- ions coming out of aqueous solution, where the ions have to shake off at least some of their salvation shells of water molecules before can attach themselves to the ionic surface layers. Other simulational approaches especially those based on Kinetic Monte Carlo method were also considered, but there was no experimental guidance available to build the model to describe interactions between the molecular constituents of the system. Therefore, this line of research was put on hold for that guidance to appear.

Kim Pihlström was a second year undergraduate when he undertook this work. It was a remarkable achievement that he did so much in a summer project. Clearly this was a valuable learning experience in which he gained experience of the strengths and limitations of molecular dynamics as a tool for modelling atomic-scale processes in these biological systems. The project gave him a taste for simulation and he has returned to carry out more simulations with other members of staff at LCE interested in biological systems finishing his M.Sc. thesis on simulating liquid drop spreading on patterned surfaces spring 2007.

Joule heating in current carrying nanowires

The focus of this project was on the theoretical techniques that have been proposed to describe the transfer of energy from excited electrons, such as those involved in current flow, to cold ions. This is a central issue in nanoelectronics because the Joule heating of current-carrying nanowires affects their mechanical stability, both by enabling thermally activated processes such as bond-breaking, and by facilitating mass transport through electromigration.

Horsfield and coworkers have shown that modeling Joule heating with traditional mean-field methods results in suppressed heating [28]. They argued that there are two reasons for this: the classical ions cannot undergo quantum excitations, and more importantly, the electronic mean-field approximation includes no information about correlations between individual electrons and ions. In order to model Joule heating, and other systems where the transitions between Born-Oppenheimer surfaces are essential, Horsfield and coworkers have developed a new modeling technique called Correlated Electron-Ion Dynamics (CEID) [29,30]. This method extends the traditional methods by allowing the ions to have quantum mechanical properties, and the electrons are no longer treated as a structureless "electron fluid". Simulations [29] show that CEID does not suffer from suppressed Joule heating. An alternative to CEID is the surface hopping method, which is a technique that has been developed to describe simple non-adiabatic processes and is able to treat heating [31,32]. Starting from classical mechanics Prezhdo and others developed an extension of classical mechanics called quantized Hamilton dynamics (QHD) [33,34,35], which adds quantum mechanical properties like zero point energy and tunnelling to classical systems. Later the QHD method was extended to include the interaction between quantum mechanical mean-field electrons and partially quantum mechanical ions [36]. This method is known as Quantized Mean-Field theory (QMF). Brooksby and

Prezhdo noted that in their test simulations the energy exchange between light and heavy particles was grossly underestimated [36], but the reason for this was unclear.

The QMF method is a hybrid between the traditional mean-field methods and CEID. We showed [15] that QMF is not able to describe Joule heating in a short nanoconductor because of the mean-field approximation used for the electrons. This result held despite the partially quantum mechanical nature of the ions in QMF bringing some improvements to traditional mean-field (i.e. Ehrenfest) simulations. In addition, we transformed [15] the QMF equations to the density operator formalism and showed that QMF is a special case of CEID.

The significance of this work is that it further underscored the need to abandon mean-field treatments of the electron gas in which the electrons are viewed as a structureless fluid in order to model Joule heating. It is only by treating the ions as quantum particles whose motions are correlated with those of the electrons in which they are immersed that Joule heating may be simulated. This message is still not adequately appreciated by many (most?) researchers in the field of nanoelectronics. For example it completely undermines the use of codes such as OCTAPUS, which is based on Ehrenfest dynamics within time-dependent density functional theory, to model Joule heating in nanoconductors. The need for CEID and methods like it is physically very transparent and cannot be stressed enough.

Jussi Kumpula carried out this research for his Masters project in Physics finishing his M.Sc. degree in 2005. It was an outstanding piece of work, at the forefront of the subject, producing one paper [15] in a good journal. After a short break M.Sc. Kumpula returned to LCE to do Ph.D. studies on Complex Systems and Networks.

Silicon interfaces and amorphous silica

As part of his PhD research Sebastian von Alfthan investigated grain boundaries in silicon. The background to this work is the experimental observation that in many commercially important ceramic systems the grain boundaries are associated with a somewhat disordered nanometre scale film. This is true in structural ceramics such as silicon nitride and in functional ceramics such as STO and BTO. In the 90s it was claimed by some simulators that the structures of high-angle twist boundaries in even pure Si are similarly disordered *in their ground states* at absolute zero. This view was very controversial, but subsequent studies seemed to confirm the conclusion that disordered atomic configurations of high-angle twist boundaries in Si have a lower energy than ordered configurations. We felt it was important to investigate this claim carefully, because it undermined decades of earlier work on the structure of grain boundaries in elemental crystalline network solids. It also raised fundamental questions about the physics of interfaces in network elemental solids which had to be settled convincingly before any real progress with the more complex alloys could be made.

We added two new ingredients to the simulation of these boundary structures. The first was that we recognised that it was essential to remove atoms from the boundary plane to access configurations that could not be generated by any other means. Furthermore, we recognised that the removal of atoms could and should be done systematically. Secondly we annealed the structures we generated for up to 100 times longer than earlier molecular dynamics simulations. Both of these new aspects turned out to be crucial to our results. We found *new ordered configurations* for the structures of these boundaries in their ground-states at absolute zero, with *lower* energies than any of those obtained by previous workers with the same potentials for Si. We confirmed the validity of our structures and the ranking of their energies by first principles density functional simulations. This work has been published in PRL [16] and PRB [17] and it has made a major international impact. We gave invited talks on this work at MMM2006 in Freiburg and the satellite COST P19 meeting in Wroclaw. We will also give an invited talk at the iib2207 meeting in Barcelona in July 2007.

A further paper is now in preparation where the influence of heating these boundaries to the melting point will be described. Again our results are quite different from those before us because we start from an ordered configuration at absolute zero and observe how it gradually disorders as it is heated to the melting point.

Sebastian defended his thesis very successfully in December 2006 and passed with distinction. The external examiner (opponent), Professor M W Finnis from Imperial College, described his work as a comprehensive demolition of the earlier claims of disordered ground-state structures of boundaries in Si, and noted that his thesis had "raised the game".

Micromechanics and optics

During this project, the Micronova clean room facility was equipped with a new atomic layer deposition reactor which allowed the development of various novel microsystems, which can utilize the special property of ALD, the conformal growth. Various micromechanical sensors are commonly used to detect very weak forces. Of special interest is to create sensor systems that are extremely sensitive to accumulated organic or inorganic mass. Since the ALD reactor is run in short cycles, one can control the final coating of the surfaces with the precision that is close to one atomic level. For organic fibers this method is very applicable since even complicated surface topographies become coated which is in practise never the case in many other growth methods. In order to test this method, we used very high-sensitivity sensor [20,37] that we originally developed to measure forces at very short distances from the surfaces (Casimir and van der Waals forces). The idea is actually quite simple, instead of using cantilevers that are used in AFM's we developed a sensor that is approaching the surface with minimum tilt so that very short distances become accessible with large detection area so that weak forces become measurable. ALD coating was an appropriate method to get control at the atomic level. Optical measurements were performed to test the quality of the sensors and on the other hand the quality and control of the ALD growth using aluminium oxide. As a side result of this project we could establish the process parameters to control the reflectivity of the surfaces with very high precision, so that anti-reflection coatings can be tailored with Al_2O_3-ALD [18]. As an example, the reflectivity of silicon surface could be controlled with extremely high precision which is believed to be useful for example in laser treatment of organic systems.
For measuring the mass of organic and other nanoscale objects we developed both very high sensitivity sensors utilizing mechanical resonances with extremely high quality (Q) factor [19,20,21] and an optical method to convert very small displacements to the shift in the rotation of laser light polarization in a cavity [22]. These results lead to the doctoral thesis of Ossi Hahtela, which is to be finished during the year 2007.

3 International Aspects

HBBG has been collaborating closely with the group supervised by prof. Ole G. Mouritsen (MEMPHYS, Department of Physics, University of Southern Denmark, Odense, Denmark). The characterization of the cytochrome c fibrils by AFM was conducted at MEMPHYS, in collaboration with DR. Adam Cohen Simonsen and Prof. Ole G. Mouritsen.

When this project started professor Adrian Sutton, FRS was dividing his time (half-and-half) between professorships at Oxford University Materials Science Dept. and LCE at TKK. From the beginning of 2005 he started as professor of physics (nanoscience) at Imperial College London, in which capacity he continued to co-supervise undergraduate and graduate student and as key-international partner of this project and bringing his international network including researchers from Oxford, Cambridge and Imperial College for the benefit of the project.

In addition, it should mentioned that Sebastian von Alfthan won in 2005 a three months internship in annual CCMS Summer Institute at Lawrence Livermore National Laboratory being one of the internationally very tightly selected 20 internship holders.

4 Publications and Academic Degrees

Table 2. Publications and academic degrees produced in the project. Numbers of different types of publications are given along with the reference numbers. List of refereed journal articles are given in Section 6.1, refereed conference papers in Section 6.2, monographs in Section 6.3 and theses in Section 6.4.

Partner	Type of publication	2003	2004	2005	2006	**Total**	Publication numbers
OEL	Ref. journal art.	1	2	1	3	**7**	6-12
	Ref. conf. papers	-	-	-	-	**-**	
	Monographs	-	-	1	-	**-**	23
	Doctoral dissert.	-	-	-	(1)	**-**	24
	Licentiate degrees	-	-	-	-	**-**	
	Master degrees	-	-	-	-	**-**	
LCE/TKK	Ref. journal art.	-	1	1	3	**5**	13-17
	Ref. conf. papers	-	-	-	-	**-**	
	Monographs	-	-	-	-	**-**	
	Doctoral dissert.	-	-	-	1	**1**	26
	Licentiate degrees	-	-	-	-	**-**	
	Master degrees	-	-	1	-	**1**	27

MQS/TKK	Ref. journal art.	-	1	2	(2)	**5**	18-22
	Ref. conf. papers	-	-	-	-	**-**	
	Monographs	-	-	-	-	**-**	
	Doctoral dissert.	-	-	-	(1)	**(1)**	25
	Licentiate degrees	-	-	-	-	**-**	
	Master degrees	-	-	-	-		
HBBG/UH	Ref. journal art.	-	1	1	2	**4**	1-4
	Ref. conf. papers	-	-	-	-	**-**	
	Monographs	-	-	-	-	**-**	
	Doctoral dissert.	-	-	-			
	Licentiate degrees	-	-	-	-	**-**	
	Master degrees	-	-	-	-		

6 Publications

6.1 Refereed Journal Articles

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6.3 Monographs

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The Research Programme for Future Electronics (TULE) was carried out between 2003 and 2006 to promote long-term and high-level basic research leading to new innovative applications, and to support the ongoing research and development effort within the Finnish electronics and electrical industry. At the same time, the programme was aimed at supporting the development of research environments within university units in order to improve researcher training opportunities. Finally, the programme hoped to encourage science students working in fields such as physics, chemistry and mathematics to turn their attention increasingly to industrial applications.

This publication is a collection of research reports by 17 projects under the TULE umbrella. In addition to showing achievements within the programme, the reports give an overall picture of the advancement and scientific level of electronics research in Finland.

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