

# GMe Forum 2008

# Abstracts of the Invited Presentations

Vienna University of Technology November 13 and 14, 2008

Society for Micro- and Nanoelectronics Vienna, 2008

Society for Micro- and Nanoelectronics c/o Institute of Sensor and Actuator Systems Vienna University of Technology Gusshausstrasse 27–29/366 A-1040 Vienna, Austria

# Thursday, November 13, 2008

10:00 - 10:30	Welcome, Coffee
10:30 - 11:00	Opening (E. BERTAGNOLLI, K. UNTERRAINER)
	Sensors:
11:00 – 11.45	B. JAKOBY: Miniaturized Sensors and Sensing Systems for Liquid Media
11:45 – 12:30	H. BRÜCKL: Magnetic Lab-on-a-Chip: Magnetic Nanoparticles for Biomedi- cal Diagnostics
12:30 - 14:00	Lunch Break
	Nanostructures and Nanotechnology:
14:00 – 14:45	M. MÜHLBERGER: Nanoimprint Lithography
14:45 – 15:30	T. PICHLER: Tailoring Carbon Nanostructures: Unravelling the Electronic Properties of Low-Dimensional Quantum Solids
15:30 – 16:00	Coffee Break
16:00 – 16:45	D. GRÜTZMACHER: Novel Device Concepts and Strategies Basing on SiGe Nanostructures
	Novel Materials and Devices:
16:45 – 17:30	P. HADLEY: Solution-Processable Electronics
17:30 – 17:45	Break
17:45 – 18:30	L. FREY: Engineering of Dielectric Materials for Silicon Technology
	The Society for Micro- and Nanoelectronics (GMe):
18:30 – 18:45	K. UNTERRAINER: Presentation of the Activities of the GMe

# Friday, November 14, 2008

#### **Opto-Electronics and Photonics:**

09:30 – 10:15	S. TASCH: LEDs for General Purpose Lighting
10:15 – 10:45	Coffee Break
10:45 – 11:15	S. SCHARTNER: Photonic Engineering of Intersubband Devices
	Sensors:
11:15 – 11:45	M. VELLEKOOP: Integrated Cell Analysis Devices
	Spintronics:
11:45 – 12:15	A. BONANNI: Origin and Control of Ferromagnetism in Magnetically Doped Nitrides. The Case of (Ga,Fe)N
12:15 - 14:00	Snacks and Poster Exhibition
	Novel Materials and Devices:
14:00 – 14:30	S. ABERMANN: New Materials and Devices for Future Generation CMOS Technologies
14:30 – 15:00	M. BREHM: Investigations on the Wetting Layer and the Island Nucleation in the SiGe System on Planar and Pre-Structured Si(001) Substrates

### Miniaturized Sensors and Sensing Systems for Liquid Media

# B. Jakoby<sup>1</sup>, E.K. Reichel<sup>1</sup>, F. Lucklum<sup>1</sup>, B. Weiss<sup>2</sup>, C. Riesch<sup>3</sup>, F. Keplinger<sup>3</sup>, J. Kasberger<sup>4</sup>, W. Hilber<sup>1</sup>

<sup>1</sup>Institute for Microelectronics and Microsensors, Johannes Kepler University Linz, Linz <sup>2</sup>Institute of Fluid Mechanics and Heat Transfer, Johannes Kepler University Linz, Linz <sup>3</sup>Institute of Sensor and Actuator Systems, Vienna University of Technology, Vienna <sup>4</sup>Integrated Microsystems Austria, Wiener Neustadt

One of the major research targets in our recent research has been the sensing of physical liquid parameters by means of miniaturized sensors. Such sensors and sensor systems can be utilized in applications, where liquids in industrial processes are monitored in order to maintain the quality of a process or the associated product. Due to the adverse properties commonly associated with chemical interfaces (lacking reversibility, drift, etc.), we concentrate our research on physical parameters as indicators for the state of the liquid, in particularly density, viscosity (or more general rheological properties), and infrared absorption. The miniaturization of suitable sensor principles facilitates the implementation of these devices online. At the same time, scaling effects have to be taken into account, which, e.g., in case of viscosity sensors, lead to issues when it comes to applications in complex liquids such as suspensions.

In our contribution we provide an overview on our recent work discussing the device design, the associated modeling, and the application of the devices.

# Magnetic Lab-on-a-Chip: Magnetic Nanoparticles for Biomedical Diagnostics

H. Brückl, J. Schotter, N. Kataeva, A. Shoshi, O. Bethge, S. Schrittwieser

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Recent progress in fabrication and characterization of magnetic nanoobjects like rods and beads has triggered many ideas and possible applications in the biomedical field. A magnetic biochip using the combination of both magnetic nanoobjects as markers and magnetoresistive sensors has proven to be competitive to standard fluorescent DNA-detection at low concentrations. Superparamagnetic nanoparticles are detected via giant magnetoresistance (GMR) or tunnel magnetoresistance (TMR) sensors. Their size ranges from a few nm up to few 100 nm and can be reliably reproduced by physical or chemical processes.

Magnetic nanoobjects additionally provide the unique possibility to actively manipulate biomolecules, on-chip, which paves the way to an integrated 'magnetic lab-on-a-chip' combining detection and manipulation. Manipulation can be accomplished either by an external magnetic field or on-chip via currents running through specially designed line patterns on a chip platform. It can be shown that hybridization processes can be accelerated compared to usual thermal activation. A prototype is under development for Sepsis diagnosis. The ultimate goal is the detection of antibodies at the picomolar level at shortest reaction times.

Today's lab-on-a-chip systems are designed in such a way that surfaces play a major role, either as substrate where molecular reaction takes place or as sensor environment for detection, combined with microfluidics. This makes them complicated, slow, and ineffective. Looking forward, a paradigm shift from the 'magnetic lab-on-a-*chip*' to a 'magnetic lab-on-a-*bead*' is discussed as a future device solution. Ferromagnetic nanoobjects are thereby directly used as both molecular recognition sites and detection units. Information about binding events is communicated via characteristic property changes of the nanoobjects which are remotely detected. For this, we envisage a combination of magnetorelaxation and plasmon detection. Symmetry considerations and numerical estimations show that anisotropic magnetic core-shell nanoobjects are best suited for this task. Au-decorated iron oxide nano-spindles were synthesized and investigated for such purposes.

# Nanoimprint Lithography

#### M. Mühlberger, I. Bergmair, W. Schwinger, M. Chouiki, H. Wiesbauer, H. Leichtfried, R. Schöftner

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Nanoimprint Lithography (NIL) is an emerging nanoreplication technology with the potential for high throughput and low cost for a huge variety of applications. The basic idea is to have a stamp which contains a (nano-) pattern. This pattern may be binary but can also contain different height levels, curved or sloped featured (e.g. microlenses), etc. In a typical nanoimprint process this stamp is then pressed into a soft material which is coated on a substrate. This soft material can be a UV-curable material but also a thermoplastic one. After UV-curing or cooling down below the glass transition temperature the stamp is removed from the now hardened material, which then features the reverse topography of the stamp. Postprocessing steps like reactive ion etching may follow, however the structured polymer can also already be the finished device.

Since the first proposal by Richard Feynman in his famous lecture "There is plenty of room at the bottom" (1959) and the first publications of S. Y. Chou [1,2] Haisma [3] and Xia [4] in the mid 1990ies a lot of progress has been made as far as equipment, processes and materials are concerned. Hot embossing or thermal NIL (using a thermoplastic polymer), UV-NIL (utilizing a UV-curing polymer) and micro- or nano-contact printing ( $\mu$ /n-CP, where an ink is transferred from the stamp to the substrate) are three variants of the same basic nanoimprint idea.

There are several important issues in a nanoimprint process that will be briefly discussed: the importance of the stamp and the stamp material, adhesion issues of the imprint material, especially in connection with the removal of the stamp from the substrate, the residual layer thickness and alignment.

Showing several examples the advantages of NIL such as high resolution patterning, multilevel patterning and direct patterning of functional materials will be highlighted.

Finally industrial applications will be discussed.

- [1] Chou, S.Y., R.P. Krauss, and J.P. Renstrom, Imprint of sub-25 nm vias and trenches in polymers. Applied Physics Letters, 1995. 67(21): p. 3114-3116.
- [2] Chou, S.Y., P.R. Krauss, and J.P. Renstrom, Nanoimprint lithography. Journal of Vacuum Science & Technology B, 1996. 14: p. 4129-4133.
- [3] J. Haisma, M. Verheijen, K. v. d. Heuvel, and J. v. d. Berg, Mold-assisted nanolithography: A process for reliable pattern replication. Journal of Vacuum Science & Technology B, 1996. 14: p. 4124-4128.
- [4] Y. Xia, E. Kim, M. Mrksich, and G. M. Whitesides, Microcontact Printing of Alkanethiols on Copper and Its Application in Microfabrication. Chem. Mater., 1996. 8(3): p. 601-603.

# Tailoring Carbon Nanostructures: Unraveling the Electronic Properties of Low-Dimensional Quantum Solids

#### **Thomas Pichler**

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The presentation will give an overview on our current research focus on the electronic properties of low dimensional quantum solids. These properties are strongly influenced by basic correlation effects. Archetypical examples of these systems are graphene, graphite and single wall carbon nanotubes (SWCNT) which are determined by the local arrangement of their sp<sup>2</sup> hybridised carbon atoms, such that their character is either semi-metallic, insulating, semiconducting or metallic. Examples of the recent work on how one can analyse these electronic properties using high energy spectroscopy (electron energy-loss, photoemission and xray absorption spectroscopy) as a probe will be presented. Special emphasis will be given to the influence of basic correlation effects and local field corrections on the electronic properties of graphene, graphite and SWCNT. The latter exhibit for metallic tubes a Luttinger liquid behavior.

Furthermore, an overview on how to functionalize nanotubes in order to tailor their electronic structure will be given. This includes examples for the three alternative doping routes, namely, substitution, intercalation and endohedral doping (e.g. by filling with fullerenes and metallocenes) as well as examples for the growth of defined innertubes from the different precursors via a thermal nanochemical reaction. In comparison to graphite intercalation compounds, the electronic structure of doped graphene will be unraveled and for metallic functionalized nanotubes doping induced changes will be discussed in the framework of a dimensionality crossover which causes a change from a one-dimensional metal to a normal Fermi liquid. The detailed understanding of these fundamental electronic properties of functionalized graphite, SWCNT and graphene is key to their future success.

# Novel Device Concepts and Strategies Basing on SiGe Nanostructures

#### **Detlev Grützmacher**

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The development of the CMOS technology in the last decade has shown that classical materials in CMOS technology materials and device principles have been exhausted, long before the ultimate physical limits have been reached. As a consequence, some materials such as HfO<sub>2</sub> as gate dielectrics and Cu as interconnect metal, which have been off limits only a few years ago, have already entered the major Si device fabrication facilities. Today, additional materials are being investigated, with a particular emphasis on hybrid systems as well as on surfaces and interfaces. While further downscaling in combination with intensified research on hybrid systems will permit the continuation of the CMOS technology path for the next 10 to 15 years, radically new approaches are required for the "beyond-CMOS" scenarios, including device principles and matching architectures.

The introduction of Ge into Si technology permits the modification of the structural, mechanical and electrical properties. Thus the implementation of Ge into Si technology leads to the design of novel devices as well as to new routes for the fabrication of nanostructures. A central challenge for nanotechnology aiming towards nanoelectronics, nanomechanics, biochemical sensors and nanophotonics is to implement exact control in the positioning and size of semiconductor nanostructures. Here, we focus on the templated self-assembly of SiGe nanostructures and discuss two pathways for the fabrication of them.

Templated self-organization of Ge dots is achieved by patterning Si substrates by extreme ultra-violet interference lithography (EUV-IL) using diffractive optics. This method offers fast large area exposure of templates with close to perfect periodicity. Si substrates have been patterned with 2-dimensional hole arrays using EUV-IL and reactive ion etching. Subsequently, molecular beam epitaxy was employed to grow Si/Ge quantum dot stacks. This process allows the fabrication of 2- and 3-dimensional quantum dot crystals containing Ge dots in a Si host crystal of unmatched structural perfection as proven by X-ray diffractometry. The Ge dots exhibit a remarkably narrow size distribution and close to perfect ordering. 2-d ordered quantum dot arrays with lateral periodicities of 50 - 100 nm as well as stacking of those quantum dot arrays into 3-d quantum dot crystals with a vertical periodicity of < 10 nm have been investigated. The results were interpreted by comparison with model calculations using nextnano3.

In the second approach Si/SiGe as well as Si/SiGe/Cr hybrid layered structures are patterned by standard lithographic techniques into mesa structures. Underetching of the mesa structures leads to a scrolling of the layer stacks into nanotubes, nanospirals and other 3-d objects due to the strain. Thus, by this technique nanostructures are produced from templates in a self-assembled fashion. The mechanisms controlling the scrolling process were analyzed in detail and their dependence on the shape, the orientation and the size of the mesa pattern was determined. Moreover, the mechanical properties of tubes, spirals and rings have been studied. Individual structures have been cut off from the substrate by micromanipulation and were subject to analysis.

Possible applications for quantum dots and scrolled nanotubes for nanoelectronic devices and nano-electromechanical systems will be discussed.

#### Solution-Processable Electronics

#### **Peter Hadley**

Institute of Solid State Physics, TU Graz

In ambient intelligence applications, the environment is filled with sensing elements, communication elements, and display elements. All of these require solution processable electronics that can be printed cheaply on substrates like plastic, cloth, or paper. Solution-processable semiconductors often have a complicated microstructure that has been difficult to control and to understand. However, our ability to determine and control the microstructure is rapidly improving. The Institute of Solid State Physics at the TU Graz has a strong program on organic semiconductors and their use in sensors, light emitting diodes, lasers, and transistors. Roland Resel described the structure of a self-assembled layer of molecules that form the channel of a transistor. His collaborators at Philips have made integrated circuits consisting of hundreds of these transistors. In Nature Photonics, a team lead by Emil List and Joachim Krenn explained how metal nanostructures can be used to efficiently extract and manipulate light from organic light emitting diodes. The fundamental crystal growth mechanisms of large organic molecules recently appeared in Science in a paper by Adolf Winkler and his collaborators in Leoben. The inside cover of the August 18th issue of Advanced Materials features an organic transistor that can be used as a chemical sensor. This transistor and its chemically active layer were built studied by Egbert Zojer and his team. The papers mentioned here represent the best of a broad effort in solution processable electronics that will contribute to the development of distributed sensors, electronic books, lighting panels, displays, solar cells, and RFID technologies. Strategies will be discussed for using inorganic materials (including silicon) in solution based processes.

# Engineering of Dielectric Materials for Silicon Technology

**Lothar Frey** 

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Scaling of electronic devices, especially of CMOS devices, follows Moore's law for more than two decades. But today, severe difficulties related to fundamental physical effects in ultra thin layers and small lateral structures have emerged. Among them are increased leakage currents and fast degradation of device parameters. One approach to overcome these problems is the introduction of new materials with specific tailored properties. Therefore, silicon technology, which was built on a rather restricted set of materials, has opened itself to a variety of new materials.

The most prominent case is probably the replacement of the gate dielectrics, silicon dioxide, by so called high k materials. In this talk, the problems related to the introduction of these new high-k materials will be discussed. The permittivity of high-k layers like Hf, Zr, or Ti based oxides is the driving force to use them in CMOS transistors to increase device performance like current drive. But in order to utilize those layers, many other problems occur and have to be solved. Examples are threshold voltage shift, mobility degradation, or parameter instability. Also new process steps like Atomic Layer Deposition had to be introduced and developed, mainly to control interfaces on sub-monolaver scale. Today, new high-k dielectrics are engineered materials with tailored properties for specific applications. High-k based gate stacks require well controlled interface and layer formation to ensure high carrier mobility, low and symmetrical threshold voltages, and tolerable degradation. After discussing this approach for MOS transistors, the application of tailored high-k dielectrics in DRAM capacitors and Flash memory cells will be shown. In DRAM capacitors, leakage current and dielectric integrity are the main issues to be engineered. On the other side, floating gate flash memory cells require controlled band alignment and low parasitic trapping in order to improve device performance.

Finally, a short outlook will show that new materials, engineered for specific electronic parameters, will open a variety of new option for scaling of classical devices as well as for heterogeneous integration of electronic components.

### **LEDs for General Purpose Lighting**

#### Stefan Tasch

Ledon Lighting Jennersdorf GmbH Technologiepark 10, A-8380 Jennersdorf

Until a few years ago, LEDs were mainly seen as low-power light sources in indicators and advertising. With huge progress being made in terms of device performance, this has profoundly changed.

Especially since the beginning of the 21<sup>st</sup> century, LED components manufacturers and material suppliers have achieved remarkable progress in their endeavor to increase chip performance, phosphor efficiency and overall device efficiency, resulting in increased luminous efficiency (lm/W), high reliability / lifetime, high color rendering etc., making solid state lighting (SSL) not only feasible for professional lighting such as displays, signage, indicators, architectural, surgical and automotive applications, but bringing it closer to enter the general lighting market with applications such as home, office, and retail lighting.

In indoor applications, fluorescent lamps are still standard, with an efficiency of 80 - 90 Im/W; however, LEDs are catching up quickly. While the efficiency of standard high-power white LEDs on the market is about 40 - 70 Im/W, efficiencies of >100 Im/W have been achieved, and LEDs with an efficiency comparable to fluorescent lamps are to enter mass production.

Besides energy saving, one big advantage of LEDs is their tunability of the color temperature. For instance, for RGB-devices, the color locus can be varied anywhere within the color gammut by independently controlling the current for R, G, and B. Furthermore, it is recognized that color rendering and color temperature have a physiological influence on humans. A combination of a blue LED with green and red phosphors would cover most of the visible spectrum and can achieve color rendering indices (RA8) of well over 90. By combination of warm and cold white devices with the appropriate drivers and sensors, it is possible to automatically adjust the color temperature with daytime and season (cold white in summer/daytime, warm white in winter/evening). Due to the potential of miniaturization, LEDs have a considerable advantage over other light sources for including optics and achieving well-defined emission angles and shapes, which would not be possible with big-sized fluorescent lamps.

#### **Photonic Engineering of Intersubband Devices**

S. Schartner, E. Mujagić, L. K. Hoffmann, B. Basnar, H. Detz, W. Schrenk, A. M. Andrews, P. Klang and G. Strasser

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Intersuband devices make use of designable quantum states within e.g. the conduction band of semiconductor heterostructures. Given a conduction band offset of a few hundred meV for most commonly used material systems such as GaAs/AIGaAs or InGaAs/InAIAs realizable transitions for optical devices range in the mid-IR region (around 10  $\mu$ m wavelength). Compact semiconductor sources as wells as detectors have been realized from 3  $\mu$ m wavelength up to the THz regime within the same concept of quantum cascade lasers (QCLs) and quantum well infrared photodetectors (QWIPs).

QCLs and QWIPs have experienced significant progress over the last decade and especially devices operating in the mid-IR region are right now at the border to commercial availability. In this respect issues such as beam quality and spectral purity gain growing interest as well as surface emitting devices since they are compatible to low cost, planar semiconductor technology.

As an adequate resonator scheme we present ring-type resonators holding  $2^{nd}$  order gratings on top. These naturally comprise both: a circularly, symmetric far field and a low beam divergency. Fabricated lasers operating in single-mode at 4  $\mu$ m wavelength have beam divergencies down to 3°.

Another related topic that needs additional attempt is the relatively low coupling of 2<sup>nd</sup> order DFB QCLs requiring long gratings and hence hindering device minimization. By switching to a different waveguide concept we were able to increase coupling and to fabricate surface emitting QCLs operating in single mode at a length a factor of 10 smaller as state-of-the-art devices.

As an alternative approach we investigate photonic crystals (PhC) since they are promising candidates for cavities used in the detecting as well as the emitting regime. Our group has developed a PhC characterization tool for mapping the photonic band structure by incorporating a QWIP in a 2D PhC. At the same time the work represents the first realization of a PhC-QWIP and delivers first experimental results showing how PhCs could potentially be used to improve detector performance.

Two more examples of novel photonic engineering realized in our group will be presented: Ycoupled cavities merging two laser ridges into one have been investigated in detail concerning their coupling behavior. The results where used to fabricate tree-lasers where more ridges are merged. This scheme is of special interest for high power, cw and/or multicolor applications. We will also present the application of chromatic cladding materials on QCLs that allow tuning the emission frequency upon changes in the ambient pH-value. In this way a transducer was realized transforming a chemical quantity directly into an optical signal.

# Integrated Cell Analysis Devices

#### Michiel J. Vellekoop

Institute of Sensor and Actuator Systems, Vienna University of Technology

The increased interest of biotechnologists to learn more about the functioning of cells has resulted in various research projects where microdevices and some times nanodevices are investigated to yield information from cells. The miniaturization of the analysis chambers and the integration of microsensors and -actuators allow new measurement techniques and new insights.

Two developments are visible; the analysis of single cells suspended in a buffer fluid, and the analysis of cell cultures that are, however, much smaller than the classical culture which contains millions of cells. Small cell cultures roughly contain less than one million cells and are grown on a sensor chip. The advantages of studying single cells and small cultures are technical; the origin and the initiation of diseases for example can be better examined, but also costs can play a significant role because of the small amount of cells and chemicals needed. For several applications it is investigated whether physical and electronic analysis methods can be used to study cells and cell behavior. Optical, electrical, magnetic, and thermal properties are examples of physical effects that are being used.

Microfluidics has become an important field in on-chip analysis devices for the control of gases and liquids that contain the cells or chemicals to treat or nurture the cells. In this contribution an overview will be given of cell analysis devices that are explored at the Institute of Sensor and Actuator Systems.

### Origin and Control of Ferromagnetism in Magnetically Doped Nitrides – The Case of (Ga,Fe)N

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<sup>4</sup> Institute of Physics, Polish Academy of Sciences, PL-02-668 Warszawa, Poland

The puzzling nature of the high-temperature ferromagnetic response lately discovered in a number of wide-band gap semiconductors and oxides has become one of the most controversial topics in nowadays materials science and condensed matter physics. Measurable spontaneous magnetization has been found in materials doped with transition metals or rare earths, and even in nominally undoped systems. Interestingly, in many cases the presence of ferromagnetism has been explained by *ab initio* computations, whose results emphasize a possible role of spin-carrying defects.

In order to shed new light on the origin of high  $T_c$  ferromagnetism, we have undertaken studies of MOVPE-grown (Ga,Fe)N, either undoped or co-doped with Si or Mg, combining the magnetic (SQUID), magnetooptical, and XANES investigation with a comprehensive structural and chemical characterization (SIMS, TEM, EDS, synchrotron XRD), which provides information on the Fe distribution at the nanoscale.

In this talk, we first discuss our quantitative study of the exchange coupling between the spins S = 5/2 localized on the Fe ions and the effective mass electrons. Our results point to an anomalous exchange splitting of the valence band, which we explain in terms of a strong renormalization of the extended states by isoelectronic impurities, specific to nitride and oxide diluted magnetic semiconductors as well as to highly mismatched alloys, like Ga(As,N).

We then show that – depending on the growth conditions and parameters – the Fe ions are incorporated into the nitride matrix in a way that gives rise to a system either diluted, or presenting spinodal decomposition in regions more or less rich in the magnetic component or showing the formation of ferromagnetic nanocrystals. In the perspective of testing the possibility to control the aggregation of the magnetic ions in a semiconducting host through the tuning of the Fermi level, we describe the effect of the Ga flow rate during growth on the Fe incorporation, which allows – when appropriately mastered – a control of the solubility limit of the transition metal ions in GaN. Moreover, the analysis of the effects of co-doping with acceptors (Mg) and donors (Si) on the magnetic behavior of the (Ga,Fe)N system, guides us to conclude that the Coulomb interaction between magnetic ions is indeed tunable via co-doping, with dramatic and controllable effects on the aggregation of the Fe-rich nanocrystals and of the regions of spinodal decomposition.

The novel mechanism of nano-self-organization that we present promises to result in new multi-component semiconductor/magnetic systems, whose characteristics and functionalities can be tuned over a wide range by fabrication parameters, co-doping, and substrate engineering.

### New Materials and Devices for Future Generation CMOS Technologies

#### S. Abermann, O. Bethge, C. Henkel, and E. Bertagnolli

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New materials and devices will be needed to continue the performance scaling for future generation CMOS technologies. The introduction of high mobility channel materials (e.g. Ge, strained Si, and III/V) on a Si-based platform, or the implementation of high-k and metal gate materials into the MOS-stack will be necessary to achieve the scaling goals as given in the International Technology Roadmap for Semiconductors (ITRS). We will present an overview of such materials and devices, including high-k/metal gate technology on high-mobility sub-strates such as Ge or strained Si, as well as new device geometry concepts.

#### Investigations on the Wetting Layer and the Island Nucleation in the SiGe System on Planar Si (001) Substrates

#### M. Brehm, M. Grydlik, H. Lichtenberger, N. Hrauda, T. Fromherz, F. Schäffler, G. Bauer

Institut für Halbleiter- und Festkörperphysik, Johannes Kepler Universität Linz

In this work, a detailed, quantitative and consistent model of the Stranski-Krastanov nucleation of SiGe islands on a SiGe (001) wetting layer (WL), grown on Si (001) substrates, is presented. Our results are based on extensive photoluminescence (PL) experiments monitoring the emission energies in the system as a function of the deposited amount of Ge with an outstandingly high resolution of 0.025 monolayers (ML) and a comparison with calculated transition energies. For all sample series investigated, the Ge layers were grown by solid source molecular beam epitaxy on 4 inch Si wafers at 700 °C. During Ge deposition the substrate rotation was switched off resulting in a gradient of the deposited Ge across the wafer diameter by  $\pm$  20% from its value at the wafer center, but otherwise identical growth conditions. Subsequent to the Ge deposition the wafers were capped with Si at three different temperatures (300 °C, 500 °C and 700 °C). For the PL investigations the wafers were cut into pieces along the Ge gradient and up to 75 PL spectra were taken on different wafer spots corresponding to different Ge contents.

An almost step-like onset of island formation at 4.2  $\pm$  0.2 ML of Ge is concomitant with an abrupt blue-shift of the WL PL signal corresponding to about 1 ML of Ge transferred from the WL to the islands during the island formation. Below this critical thickness, the WL PL shifts seemingly linear to lower energies with increasing amount of deposited Ge. This shift and its dependence on the capping layer growth temperature (T<sub>c</sub>), is quantitatively explained by calculating the PL WL transition energies based on 6-band k·p band structure calculations [1]. These calculations allow us to determine for the first time reliable Ge profiles across the WL for the different capping temperatures. At the onset of Ge island formation, the peak Ge content in the wetting layer exceeds 80% at its lower interface. Surface segregation of Ge on Si was identified as the dominant process responsible for the deduced Ge profiles. These profiles allow us to explain the observed blue-shift of the WL PL emission band with increasing T<sub>c</sub>. From a simple exponential model, a variation of the Ge-concentration decay length in the WL between 1 and 5 Å is obtained for the investigated T<sub>c</sub> range from 300 °C to 700 °C, for Ge coverages smaller than the critical one for island formation

An accurate determination of the amount of Ge transferred from the WL to the islands during spontaneous island nucleation is obtained. This determination is based on the measurement of the total island volume on uncapped reference samples by atomic force microscopy for the different amounts of deposited Ge in combination with the observed WL PL shifts. Furthermore, for this growth temperature an average Ge concentration in the islands ( $35\% \pm 2\%$ ) was obtained, confirmed by x-ray diffraction experiments and calculations of the island PL energy using the nextnano3 code [2].

- [1] M. Brehm, M. Grydlik, H. Lichtenberger, N. Hrauda, F. Schäffler, W. Jantsch, G. Bauer: "Quantitative determination of Ge profiles across SiGe wetting layers on Si(001)", Appl. Phys. Lett., 93, 2008, 121901 1-3.
- [2] http://www.wsi.tu-muenchen.de/nextnano3/index.htm