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Preface

Dear partners and friends,

it has been a long tradition at the Institute of Physics to present an annual report. But since organizational and personnel changes as well as significant scientific progress take place rather on a timescale of two years or longer, we decided to move to a bi-annual reporting scheme. This is now the first bi-annual report of the Institute of Physics, covering the research- and teaching activities from the years 2010 and 2011.

After some major personnel and infrastructural changes in 2009, the Institute has now reached a steady state situation. Adaptation of the new laboratories has been finalized in the first half of 2010, although some of the laboratories still suffer from currently not affordable experimental equipment. The personnel situation at the institute is stable at about 20 staff and additionally up to 10 students.

The faculty staff is strongly involved in teaching and examining all Bachelor students of the Montanuniversität in Physics in their first two years. Furthermore, we are very active in the Materials Science Bachelor- and Masters Curriculum, in particular within the “Wahlfachgruppe: Materials for Electronics and Physics of Functional Materials”. All in all, the Institute of Physics has delivered on average 80 hours of weekly teaching during each semester, and more than 4000 individual examinations were taken. Nine PhD theses and seven Diploma theses were supervised, thereof three PhD theses and five Diploma theses were finished within the reporting period.

In terms of external funding acquisition the Institute was quite successful. Ten research projects (5 FWF, 3 FFG, 2 DFG, with a total budget of roughly 2 Million Euro) with at least one project-financed scientific coworker were managed, thereof three projects new starting and five projects ending within the reporting period. In addition several smaller projects (ÖAAD, EU Cost-action, contract research for industry) were carried out, and several beamtime projects at large scale facilities for synchrotron radiation or neutrons were granted to members of the Institute.

The scientific mission of the Institute is to conduct high-quality basic scientific research on the physics of nanosystems and semiconductors. Actual research topics range from quantum bits to photonic crystals and from organic semiconductor thin films to nanoporous biomimetic ceramics. The last two years were exceptionally successful in terms of scientific output with more than 60 peer-reviewed articles in science citation index (SCI) listed journals. Some of them were published in high-impact journals such as *Nano Letters, ACS Nano* (2), *PNAS*, and *Physical Review Letters* (2). With more than 30 articles per year the Institute of Physics contributes currently about 15% to the total SCI-listed publication output of the Montanuniversität Leoben. The scientific reports summarizing these scientific achievements are the heart of this bi-annual report.

Besides the importance of publishing novel scientific results, also the direct scientific dialog is extremely important. Members of the Institute have presented more than 100 lectures (30 of them invited) and more than 50 posters at conferences and workshops, and have delivered 26 invited talks at seminars in external institutions. Three workshops and two international schools were primarily organized by members of the Institute, and some of us have further contributed to the success of several events as session organizers and session chairpersons. We are also particularly proud to run a very active international scientific seminar with weekly lectures on “Semiconductor Physics and Nanotechnology”. Almost 40 seminars from internationally renowned scientists were held during the reporting period 2010/2011, with half of the speakers coming from abroad. Last but not least, Igor Beinik received the “Anton Paar Wissenschaftspreis für Physik 2011” for the best PhD thesis on solid state physics in Austria.

I am very grateful to all members of the Institute for their contributions to this success story, compiled in detail in the following pages. I hope you enjoy reading through this report and keep in touch with the Institute of Physics.

Univ.-Prof. Dr. Oskar Paris

August 2012
The “handover” of the Institute of Physics from Prof. Kuchar to Prof. Paris on the occasion of their farewell- and inaugural lectures with the common title “Die Physiker: Strahlung – Teilchen - Festkörper” (The Physicists: Radiation – Particles – Solids).
1. Personnel

Faculty: Professors and Assistants

Univ.-Prof. Dr. Oskar PARIS
(Chair)

Em. O.Univ.-Prof. Dr. Friedemar KUCHAR

Ao.Univ.-Prof. Dr. Josef OWALD
(Vice-Chair)

Ao.Univ.-Prof. Dr. Ronald MEISELS

Ao.Univ.-Prof. Dr. Christian TEICHERT

Dipl. Phys. Maxim ERKO
PhD Student

Dr. Markus KRATZER
Senior Researcher

Dr. Markus HARTMANN
Senior Researcher

Dr. Rainer LECHNER
Senior Researcher

Faculty: Administration and Technical Support

Heide KIRCHBERGER
(Secretary)

Magdalena OTTRIN
(Secretary)

Peter MOHARITSCH
(Mechanical Engineer)

Ing. Heinz PIRKER
(Electrical Engineer)
Research Associates

Dr. Roland BRUNNER
Postdoc

Dr. Christoph UIBERACKER
Postdoc (until 11/2010)

Dr. Oleksandr GLUSHKO
Doctoral student (until 4/2011)

Dr. Christoph UIBERACKER
Postdoc (until 11/2010)

Dr. Igor BEINIK
Doctoral student (until 04/2011)

Dr. Gerhard POPOVSKI
Postdoc

Dr. Franz SCHMIED
Doctoral student (until 4/2011)

Dipl.Ing. Christian GANSER
Doctoral student (since 10/2011)
Diploma student (until 6/2011)

Dipl.Ing. Andreas PAVITSCHITZ
Doctoral student (since 12/2010), Diploma student (12/2010)

Dipl.Ing. Stefan LORBEK
Doctoral student (since 1/2009)

Dipl.Ing. Quan SHEN
Doctoral student (since 6/2009)

Dipl.Ing. Seyedsoran NABAVI
Doctoral student (since 10/2011)

Dipl.Ing. Lin WANG
Diploma student (since 1/2010)

Dipl.Ing. Abdellatif JERRAR
Diploma student (since 9/2011)

Stefan KLIMA
Student worker (since 1/2011)

Dipl.Ing. Nurdogan GÜRKAN
Diploma student (until 12/2010)

Roland MORAK

Dipl.Ing. Mario LUGGER
Diploma student (until 3/2012)

Christian PREHAL
Student worker (from-9/2011 to 11/2011)

Dipl.Ing. Astrid WACHAUER
Diploma student (until 6/2011)

Mladen-Mateo PRIMORAC
Student worker (from 10/2010 to 6/2011 and since 10/2011)

Christian STECHER
Student worker (until 2/2012)
## 2. Teaching

### 2.1 Courses held in the academic years 2009/2010 and 2010/2011

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#### Summer Term 2010

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**Winter Term 2010/2011**

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**Summer Term 2011**

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### Anwendung von Computersimulationen in der Metall- und Biophysik

2 VO Hartmann M

### Elektronische und mechanische Eigenschaften von Heterostruktur-Bauelementen

2 VO Kasper E

### Exkursion: Synchrotronstrahlung in der Materialforschung

2 EX Paris O

### Grundprinzipien der Quantenphysik

2 VO Oswald J

### Magnetische Eigenschaften von Nanowerkstoffen

2 VO Lechner R

### Physik II

2 VO Paris O

### Physik III

2 VO Teichert C

### Physik von Fullerenen, Graphen und Carbon Nanotubes

2 VO Teichert C

### Rastersondentechniken zur Charakterisierung von Festkörperoberflächen

2 VO Teichert C

### Rechenübungen zu Physik II (14 Gruppen)


### Rechenübungen zu Physik III (2 Gruppen)

1 UE Kratzer M, Teichert C

### Repetitorium Physik I

1 RP Paris O

### Repetitorium Physik I

1 RP Oswald J

### Seminar aus Halbleiterphysik und Nanotechnologie

2 SE Meisels R, Oswald J, Paris O, Teichert C

### Strukturforschung mit Röntgen- und Neutronenstreueung an Europäischen Großforschungsanlagen

2 VO Keckes J, Paris O

### Übungen zu Mechanisch-Physikalische Messtechnik

2 UE Meisels R, Oswald J, Schmied F

### Übungen zu Physik II (6 Gruppen)

2 UE Erko M, Hartmann M, Kratzer M, Lechner R, Meisels R

### 2.2 Lectors: External help with teaching

Teaching is usually covered by the faculty staff members. However, to cover the exercises and the practical training in Physics for the freshmen students we have to rely on the help from motivated lecturers from the research associates from the Institute of Physics and from other Chairs of the MUL. We are grateful for the help from:

- Dr. R. Brunner, Dipl. Phys. O. Glushko, Dipl. Phys. S. Lorbek, Dipl. Ing. A. Pavitschitz, Dr. G. Popovski, Dipl. Ing. F. Schmied, Institut für Physik
- Dr. M. Hofstätter, Institut für Struktur- und Funktionskeramik
- Dr. M. Milko, Dr. P. Puschnig, Lehrstuhl für Atomistic Modelling
- Dr. S. Sagmeister, Lehrstuhl für Atomistic Modelling and Materials Center Leoben
- Dipl. Ing. S. Wurster, Lehrstuhl für Materialphysik
- Dipl. Ing. W. Hyden, Lehrstuhl für Geophysik
## 2.3 Exams

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<td>Halbleiterwerkstoffe</td>
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3. Research

3.3 Research reports

Research at the Institute of Physics covers four major fields, namely surface physics, semiconductor physics, optics and electronic transport, and nanomaterials including biological and biomimetic systems. (Nano-) structure and functional properties of a wide range of materials are in the focus of current research. Two major experimental methods are employed within the Institute, namely scanning probe microscopy and X-ray and neutron scattering techniques, including the extensive use of synchrotron- and neutron radiation at large-scale facilities. Experimental work is complemented by a range of numerical simulation tools such as Monte Carlo simulations, finite difference time domain (FDTD) calculations or quantum mechanical simulations.

There are four independent research groups each lead by one of the four Professors of the Institute. The following pages compile the research reports from these groups in the reporting period 2010/2011.

**Nanomaterials and Scattering:** Oskar Paris
Maxim Erko, Markus Hartmann, Rainer T. Lechner, Soran Nabavi, Roland Morak, Gerhard Popovski, Christian Prehal, Mladen M. Primorac

**Surface Physics and Scanning Probe Microscopy:** Christian Teichert
Gerard Abdellatif, Igor Beinik, Nurdogan Gürkan, Stefan Klima, Markus Kratzer, Stefan Lorbek, Mario Lugger, Andreas Pavitschitz, Christia Prehal, Franz Schmied, Quan Shen, Astrid Wachauer, Lin Wang

**Photonics and Nanoelectronics:** Ronald Meisels
Roland Brunner, Oleksandr Glushko, Friedemar Kuchar

**Simulation Electric Transport:** Josef Oswald
Christian Stecher, Christoph Uiberacker
Physicists have long been interested in the study of fluid behavior in confined geometries. These studies are highly relevant for both, science and technology. The Physics and Physical Chemistry of gas storage for energy applications, of heterogeneous catalysis, or many aspects of life sciences are affected by fluid properties modified through nano-confinement. For instance, both, the condensation pressure and the freezing temperature of fluids scale with confinement dimensions following the classical Kelvin- and Gibbs-Thomson equations, respectively. Moreover, due to the huge internal surface of modern nanoporous materials, gas adsorption and condensation as well as liquid freezing are able to deform the solid pore walls considerably. These effects are, on the one hand, critical when drying highly porous materials such as aerogels or nanopatterned surfaces. On the other hand, they also open new avenues for sensors and actuators with unbeaten sensitivity.

1) Water properties in confined geometry

Studies of liquid water properties are essential for numerous scientific fields aiming at the understanding of the fundamentals of life. The unique structural behaviour of water has been shown to be even more pronounced upon strong supercooling. Enclosing water into nano-confinement distinctly modifies its phase diagram extending the supercooling region to temperatures as low as 200K [1]. Thus, the previously inaccessible temperature region of liquid water (“man’s land”) can be studied by enclosing water into pores with diameters smaller than ~3 nm. We performed a systematic study by employing a series of nanoporous silica samples (MCM-41 silica with ordered cylindrical pores on a hexagonal lattice) with pore diameters ranging from 4.5 nm down to 2.0 nm. We found distinct confinement effects on the bonding and ordering structure of water molecules by means of Raman scattering [2], and by a combined scattering study using synchrotron radiation X-rays and neutrons [3], respectively. Both studies reveal a non-uniform occupation of the pore volume by water molecules resulting in two distinct water phases in hydrophilic nano-confinement. They consist of a high-density water layer close to the pore surface and a core water region in the middle part of the pores with lower density (see Figure 1). A recently reported water density minimum around 210 K [4] was also found in our work. However, this minimum was shown to be influenced by the pore size, moving to lower temperature as the pore size decreases. Therefore, we conclude that this density minimum is due to the water freezing transition, and not – as speculated earlier in [4] – due to a liquid-liquid phase transition of bulk water.

Figure 1: Two water phases are present in nano-confinement characterized by a different degree of the hydrogen-bonding structure. A distinct tetrahedral hydrogen-bond network of water molecules is found only in the core part of the pores. This core water part undergoes considerable structural change with confinement dimensions leading eventually to a fully amorphous structure also at low temperature.

2) Sorption phenomena in SBA-15

SBA-15 silica has a similar structure as MCM-41, but the pores are larger (7-9 nm diameter) and the pore walls are rough and have a complex gradient structure. Sorption of fluids with different electron density in combination with in-situ SAXS can therefore be used to learn more about the pore structure itself, and the changed sorption behaviour. We have shown that not only the sorption isotherm can be calculated from the in-situ scattering data, but that these data contain considerably more detailed information on the pore wall structure [5]. Apart of the sorption behaviour of model fluids with small molecules, these materials are also ideally suited to study the adsorption behaviour of larger molecules such as proteins, lipids etc. for biomedical applications. In close cooperation with the group of G. Findenegg from the TU Berlin, we have recently studied the adsorption of surfactants in water filled SBA-15 using small-angle neutron scattering [6, 7]. Quantitative studies of phase transitions in confined geometry are experimentally challenging and time consuming due to very slow equilibration. Thus, sufficient equilibration time between the single measurements is required for systematic in-situ studies. An in-situ sorption device (Combined Scattering and Adsorption, COSCAD) was developed to study sorption processes in ordered nanoporous materials using a laboratory small-angle X-ray scattering instrument (NanoStar, Bruker AXS). As a first application of this new instrument, the long-term structural stability of SBA-15 was investigated by recording in situ SAXS patterns during repeated water sorption [8]. The study revealed irreversible changes of the silica pore matrix partially enclosing water within collapsed pore regions (see Figure 2). Modifications of porous materials upon repeated interaction with water were not considered in previous sorption studies. Hence, these first results provide an important contribution for further studies aiming at the understanding of irreversible changes during water sorption.
therefore laid on the quantitative understanding of the remain only poorly understood. A particular focus was experiment [11]. Still, there are some phenomena which the successful interplay of theory/modeling with University in Berlin [9, 10], and to an overview article on theses that were accomplished at the Humboldt the last years for different fluids and as a function of.

We have studied this phenomenon extensively within the ordered pore lattice. Figure 3 shows a sorption isotherm, i.e., the pore lattice strain as a function of relative fluid pressure during sorption.

3) Sorption strains in nanoporous materials

Adsorption of a fluid within a nanoporous system changes the interfacial energy of the pore wall and is therefore related to a surface stress of the solid. This surface stress induces a bulk stress and leads to a deformation of the solid. Such sorption strains can be measured in ordered nanoporous systems by simply calculating them from the shift of the Bragg peaks of the ordered pore lattice. Figure 3 shows a sorption isotherm, i.e., the pore lattice strain as a function of relative fluid pressure during sorption.

We have studied this phenomenon extensively within the last years for different fluids and as a function of pore size and porous system. This has led to two PhD theses that were accomplished at the Humboldt University in Berlin [9, 10], and to an overview article on the successful interplay of theory/modeling with experiment [11]. Still, there are some phenomena which remain only poorly understood. A particular focus was therefore laid on the quantitative understanding of the different parts of the strain isotherm. A careful data analysis combined with numerical and analytical modeling of the scattered X-ray intensity revealed a subtle contrast effect, which leads to an apparent strain contribution in the isotherm [12].

Cooperation

J. Prass, D. Müller (MPI of Colloids and Interfaces, Potsdam), G. H. Findenegg (TU Berlin), D. Wallacher, I. Zizak, A. Hoell, T. Hauß (Helmholtz Zentrum Berlin), N. Cade, A. G. Michette (King’s College London).

References

With the rise of powerful computers starting from the second half of the 20th century computational physics established itself as the third pillar of physics in between the traditional branches of experimental and theoretical physics. Computer simulations are widely used to perform calculations that are too lengthy, too complicated or simply not possible to be done analytically. Simulations also give the opportunity to implement theoretical model systems and to perform "experiments" on them. These computer experiments can either be designed to match real experiments to check the validity of a suggested model (this is especially important when the experiments give only indirect evidence on the underlying principles like a scattering experiment) or to conduct experiments that would not be possible in reality (like working at zero or infinite temperature). Furthermore, in a computer simulation the system is known in every detail lacking the noise and uncertainties inherent in each real experiment.

In our group we use Monte Carlo simulation techniques to investigate the structure and mechanical behavior of complex materials. These include biological materials like bone or the mussel byssus and carbon nanostructures like graphene, carbon nanotubes and fullerenes.

1) Sacrificial Bonds in Biological Materials

In the framework of the FWF project P22983-N20 the influence of sacrificial bonds on the mechanical behavior of biological tissue is investigated. Sacrificial bonds are weaker than the covalent bonds holding the structure together and they can open and close reversibly. They provide hidden lengths allowing for an efficient energy dissipation mechanism enhancing considerably the toughness of biological materials as well as allowing for self repair. Sacrificial bonds are reported in a variety of biological materials. In our group the focus is put on bone and the mussel byssus. In a first study it was shown that ionic sacrificial bonds have to be randomly distributed to provide shear deformability. Now our focus lies on the influence of sacrificial bonds on the mechanical behavior of the mussel byssus.

Fig. 1 The load-displacement curve for stretching and relaxing a polymer chain with additional sacrificial bonds. Note the pronounced hysteresis between stretching and relaxing corresponding to energy dissipation.

The investigated model consists of a covalently bonded linear chain with some monomers defined as sticky sites. Two sticky sites can form a sacrificial bond that is weaker than the covalent bonds and that can thermally activated open and close reversibly. In Fig. 1 a load-displacement curve for a simulated cyclic loading experiment on such a system can be seen. Most interestingly a pronounced hysteresis between stretching and relaxing can be observed that shows the amount of dissipated energy per loading cycle. Future investigations will include the effect of different arrangements of sticky sites (ordered, random or in patches) as well as the parallel coupling of several polymer chains that allow cross linking of these chains.

Cooperation
Matthew J. Harrington, Peter Fratzl (Max-Planck-Institute of Colloids and Interfaces, Potsdam)

References
- Markus A. Hartmann & Peter Fratzl: Sacrificial ionic bonds have to be randomly distributed to provide shear deformability, Nanoletters 9, 3603 (2009)
Carbon nanostructures are characterized by an extremely high stiffness and low weight making them a promising candidate for applications in structural mechanics. The mechanical properties of macroscopic carbon structures are strongly influenced by its properties on atomistic and nanometer length scales, especially the type, amount and distribution of defects present, like vacancies, Stone-Wales or Wigner defects. These different length scales make a multi-scale/multi-method approach inevitable when predicting the mechanical properties of carbon structures. In a joint effort with partners from the Montanuniversität Leoben and the Technical University of Vienna we combine ab initio, Monte Carlo and Finite Element methods to investigate carbon structures on a quantum mechanical, classical atomistic and continuum level.

David Holec performed ab initio calculations on graphene and nanotubes to obtain classical bond-stretching, bending and torsion potentials of perfect carbon nanostructures. These were used in subsequent Monte Carlo simulations on fullerene structures to, first, investigate the validity of the classical approximation and second, calculate the excess surface energy of fullerenes as a function of radius. It was shown that Monte Carlo simulations overestimate the excess curvature energy with a constant factor of around 1.6 but predicted the same exponents when fitted with respect to the radius. This overestimation of energy stems mostly from the fact that curved fullerenes break the symmetry of planar graphene. Bending of the structure yields a lower electron density on the inside of the structure than on the outside an effect that is not captured by classical potentials. Lastly, the Monte Carlo simulations showed that torsion energy gives by far the highest contribution to the excess curvature energy albeit its small force constant.

Whenever the system of interest is composed of many different layers, like carbon onions or multi-walled nanotubes, van der Waals interactions mediate the non-covalent bonding between adjacent layers. Monte Carlo simulations were used to validate a new continuum modeling approach to describe these interactions in carbon onions. These systems demand a special treatment of these non-covalent interactions because adjacent layers consist of a different number of atoms resulting in different pressures on neighboring layers. In the simulations we could show that the newly proposed formulation yielded considerable better results than continuum formulations that did not explicitly include curvature effects.

Current and future investigations include the mechanical properties and the role of defects (their concentration, distribution and interactions) on the mechanical properties of carbon nanostructures like graphene, nanotubes, fullerenes and carbon onions, respectively. The role of defects will be investigated by ab initio calculations to find classical potentials and subsequent Monte Carlo simulations on larger structures. Mechanical properties of these nanostructures are derived by doing computational mechanical tests on the structures, like compression tests (see Fig. 2). The outcome of these tests (compression moduli and critical pressure, respectively) will serve as input to Finite Element calculations of larger structures.

**Cooperation**
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David Holec, Paul H. Mayrhofer (Department of Physical Metallurgy and Materials Testing, Montanuniversität Leoben)
Franz D. Fischer (Institute of Mechanics, Montanuniversität Leoben)

**References**
**Nanomaterials & Scattering**

**Magnetic- and Semiconducting Functional Nanoparticles**

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A main focus of our work is the structural characterisation of nanocrystals (NCs) with small and wide angle x-ray scattering techniques (SAXS and WAXS) at laboratory- and synchrotron-sources as well as to complete these findings with complementary microscopy techniques. The detailed knowledge of the structural properties allows to study the impact of the nanometer sized dimensions on their magnetic and optical properties.

Colloidal nanoparticles are of great interest for current applications in medicine and for future data storage. Magnetic nanoparticles are used for tumour detection and treatment. In future these nanomagnets could be also ordered in 2D arrays as magnetic bits in high density memory devices. Semiconductor nanocrystals can be used as efficient detectors for the infrared in organic infrared photodiodes.

For all these applications and further developments a controlled growth of these nanocrystals is essential, and hence a basic understanding of the underlying growth mechanisms on the atomic scale.

Furthermore, using single nanocrystals as building blocks to form artificial nanocrystal solids [1] may lead to materials with new designable functionalities.

1) Core/shell structure of PbS/CdS nanocrystals measured with ASAXS and WAXS

Chemically synthesised semiconducting colloidal quantum dots are of great interest for numerous applications requiring bright and stable fluorophores, especially after stabilizing the NC-core with a hard protective shell [2]. Lead chalcogenide NCs, especially PbX with X=Se, Te, S, provide efficient emission over a large spectral range in the infrared, e.g., PbS NCs in photodiodes for the mid-infrared, but their application has been limited by instabilities in their optical performance on exposure to ambient conditions. In contrast to an epitaxial shell growth on top of the already formed core material [2], we investigate in this study the CdS-shell growth on PbS NCs driven by Cd for Pb cation exchange.

In this work, we perform anomalous SAXS (ASAXS) experiments at the beamlines ASAXS at HZB-Bessy II (Berlin) and ID01 the ESRF (Grenoble). Tuning the x-ray energy just below the Pb-LIII-edge at 13.035 keV allows to record SAXS spectra at different energies, where the contribution of Pb to the total scattering signal is varied. This allows for resolving the total electron density as well as the Pb-atom density inside the core/shell NCs independently by applying a unique core/shell spherical model to fit all 5 scattering curves (see Fig.1 a). With this method we derive the following results: During the Cd for Pb exchange process applied to 10 nm sized PbS spheres, the PbS core shrinks, the CdS shell thickness increases, while the outer diameter remains constant. The final PbS core diameter is determined to be 6.9 nm with a 0.8 nm pure CdS shell (see Fig.1 b). Pb can be only traced within the core region indicating the existing of an atomic sharp interface between core and shell. Starting with smaller PbS NCs the outer diameter remained again constant at 5.2 nm, but a very thick final shell of 1.9 nm is formed with a small reaming core of only 0.9 nm in diameter. For this shell-thickness we detect 2 Pb atoms/nm² within the CdS-shell indicating an interdiffusion profile of Pb, CdS around the remaining PbS core. We found a clear trend that the final CdS-shell thickness increases with decreasing starting diameter of the pure PbS NC. We relate these findings to an increased cationic exchange due to an increased surface to volume ratio for the smaller NCs.

Furthermore, from wide angle x-ray scattering (WAXS) compared with TEM measurements (Fig. 1c) the crystallographic properties of the PbS/CdS core/shell structure was derived. We found evidence for a crystalline metastable phase of the CdS-shell keeping in the beginning of the exchange the rocksalt structure of PbS and changing later to the CdS wurtzite structure.

**Fig. 1:** (a) ASAXS scattering curves recorded at 5 x-ray energies just below the Pb-LIII edge (symbols) together with their fits (lines) using one unique core/shell model. Inset: shift of the first minimum position for a core/shell NC (black square) and an uniform PbS NC (red) (b) resulting total electron density (blue line) and Pb density (red line) profiles resulting from a). (c) TEM image of a single PbS/CdS core-shell particle. The core is indicated by a red dashed line, the outer shell by a blue dashed line.

2) Self assembled nanocrystal solids

Colloidal nanocrystals can combine the benefits of inorganic semiconductors with size-tunable electronic structure and inexpensive solution-based device fabrication. Nanocrystal assemblies, also known as superlattices, using single NCs as individual building blocks offer the opportunity for designing artificial crystalline solids with tailored electronic, magnetic, and...
optical properties. Many technical applications will require, however, micrometer scaled nanocrystal solids formed by a controlled assembling process to ordered 2D or 3D structures.

Recent studies of nanocrystals solids revealed various crystallographic aspects (defect formation, quasi-crystalline ordering, binary and ternary structures, etc.) similar to those found in atomic and ionic crystals. We are interested in the crystalline properties of single nanocrystal solids as well as in the growth kinetics of these artificial solids formed of an ensemble of single NCs in solution.

We studied the template free self-assembled growth of nanocrystal solids made of individual 17 nm sized Bi NCs [Fig 1.(a)]. Recently Bi NC-solids with a typical size of 10 to 40 μm were grown using a slow destabilization approach. In this approach, the solution was slowly destabilized by diffusion of a non-solvent, leading to the evolution of interparticle interactions from strongly repulsive to attractive due to the change in solvent-ligand interactions.

The crystalline structure of these NC-solids was recorded in the small x-ray scattering regime (SAXS) by ex-situ single crystal synchrotron diffraction experiments. Simultaneously the atomic structure of the Bi NCs was probed in the wide angle regime (WAXS). These experiments were performed at the beamline μ-spot at the synchrotron BESSY II (HZB-Berlin).

Micrometer sized NC-solids [Fig. 2(b)] were attached by means of a micromanipulator under an optical microscope on top of a fibre tip, which is aligned in the 100x100 μm sized x-ray beam. By rotating the tip up to 360° the whole 3D reciprocal lattice space (RSM) of single Bi NC-solids can be recorded [Fig. 2(c)-(f)]. The 3D RSM in Fig. 2(c) reveals a hexagonal pattern of the Bragg peaks that could be related to a hexagonal lattice structure in real space with the c-axis parallel to the viewpoint. The 3D RSM in Fig. 2(d) is rotated 90° with respect to the c-axis revealing double streaks along the c-axis. These streaks could be caused by faults in the hexagonal ABAB stacking of single Bi-NC layers along the c-axis. From this we can conclude that the measured single NC-solids consist of two twisted hexagonal lattices. The angle between the streaks suggests a shape as shown in the SEM images of the inset between Fig.2(c) and (d).

The 3D RSMs in Fig. 2(e)-(f) originates exactly from the NC-solid as shown in the optical microscopy image (inset) depicting a hexagonal outer shape with 10 μm side length. From the RSMs we derive a hexagonal lattice constant of 16 nm and can conclude on a single hexagonal crystal structure, but with stacking faults along the c-axis.

Furthermore to study the growth kinetics of these artificial crystals, we measured in-situ at the Austrian SAXS beamline at ELETTRA the above described formation process of the Bi NC-solids. We could record the onset of the crystallization process time resolved as a function of the nanocrystal concentration. A continuing in-situ measurements with even ms-time resolution will be performed this year.

3) Magnetic semiconductor nanostructures

A further research topic is the growth and characterisation of ferromagnetic semiconductor structures in cooperation with G. Springholz from the JKU, Linz. Characterisation methods using x-ray diffraction (XRD) at synchrotrons for probing the structural properties of embedded semiconducting nanomagnets were developed together with V. Holy of the Charles University Prague [3].

Transition metal doped semiconductors, which combine ferromagnetic and semiconducting properties, have drawn large interest for possible future spintronic applications. Among these materials are magnetic IV-VI compounds like Ge_{1-x}MnxTe, for which ferromagnetic Curie temperatures of up to 200 K have been reported for layers grown by molecular beam epitaxy (MBE) [4].
Their crystalline structure and phase, however, depend strongly on the Mn concentration as well as on the growth conditions. The influence of crystallographic phase decomposition on the magnetic properties was revealed by combining synchrotron XRD, AFM and TEM investigations with SQUID magnetometry (Fig. 3). The formation of secondary phases, e.g. hexagonal MnTe in Fig. 3(b), strongly reduces the layer magnetisation. The ferromagnetism could be directly related to the cubic Ge$_{1-x}$Mn$_x$Te phase [see Fig. 3(c)-(d)]. The coexistence of antiferromagnetic MnTe and ferromagnetic Ge$_{0.5}$Mn$_{0.5}$Te, however, resulted in magnetic exchange-bias effects [5]. Under optimized conditions, single phase GeMnTe layers were obtained depicting only stacking faults with Curie temperatures as high as 200 K for Mn concentrations close to the solubility limit of xMn~50% [4, 5].

An additional in house cooperation with the group of C. Teichert encompasses the characterisation of ZnO-nanowires by means of x-ray diffraction analysis [6].

References


Nanomaterials & Scattering

Biomimetic Materials Research

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On research on biomimetic materials focused on two topics during the last two years. Both of them are related to the hierarchical structure of natural nanocomposite materials. The first topic deals with the transformation of woody plant material into ceramics on all levels of hierarchy. This is a project within the Schwerpunktprogramm SPP-1420 of the Deutsche Forschungsgemeinschaft (DFG) “Biomimetic Materials Research: Functionality by hierarchical structuring of materials”. The second topic is on the mapping of structure and composition of biological composite materials using microbeam scanning small-angle scattering.

1) Biomimetic processing

Macroscopically, spruce wood shows annular growth rings, consisting of elongated cells with a cross section diameter of some 10-30 µm. The cell walls are a composite material where fibrils are embedded into a lignin matrix. The fibrils have a diameter of about 10-15 nm and they are arranged helically around the axis of the cell wall. Within each fibril there are bundles of cellulose microfibrils, which have a diameter of about 2-3 nm. Between these microfibrils and at the outer surface of the fibrils there are different hemicelluloses.

The main aim of the work [1] was the ceramic replication of wood on all levels of hierarchy. Replication at the cell-wall level and above has already been reported in literature before, but the replication of the nanometre sized structures within the cell wall has rarely been shown. Materials synthesis using spruce wood as a template was done by our partners at the University of Erlangen, by applying various preparation schemes based on sol-gel silica synthesis. A crucial step was the delignification making the nanometre cell wall structures accessible to allow for the impregnation with tetraethyl orthosilicate (TEOS). The second important step was the modification of the material to optimize the process. This was either achieved by modification with maleic acid anhydride or a second infiltration cycle with TEOS. Heating of sample to 500°C in air (calcination) led the disintegration of the organic material, resulting in a highly porous pure silica material. Several microscopic techniques (light microscopy, SEM, TEM) and small angle x-ray scattering (SAXS) showed that the structure of wood was preserved down to the nanometer range (Fig. 1).

TEOS is believed to enter the swellable part of the structure (which is dominated by hemicelluloses), but not the cellulose microfibrils. The calcination process leaves therefore porous space where the cellulose microfibrils used to be. The resulting pores are therefore nanometre sized and chiral. A second type of macroscopic parallel pores is also created from the voids within the cell lumina. The nanopores within the template ceramics change its mechanical properties compared to a bulk ceramic. This has been tested by using nanoindentation. The reduced modulus of the wood derived silica increases from 17 GPa to 27 GPa and the hardness from 0.4 GPa to 2.7 GPa as compared to the native wood. The load-displacement curves (Fig. 2) of the native wood show a large hysteresis. This hysteresis is largely maintained in the inorganic material as compared to bulk silica, indicating the ability to dissipate a large amount of energy without breaking. This can be attributed to the nanopores, which capture propagating cracks and lead therefore to enhanced fracture toughness.

Fig. 1 Hierarchical structure of wood (left) and its silica replica (right). Upper row: light microscopy images; middle row: SEM images; lower row: SAXS patterns.
Fig. 2 Load-displacement curves of wood and of ceramics templated by wood. The blue curve shows the curve for fused silica as a reference.

Another cellulose based material that has been used as a template for the replication process was the peel of a pomelo [2]. This highly impact resistant structure consists of cells forming a foamy structure with a density gradient from the inside to the outside. The cell walls consist mainly of cellulose and other polysaccharides such as hemicelluloses and pectin. The procedure was similar to the one used for spruce wood, except that delignification of the material was not required. The resulting silica material has foam like structure with a porosity of 96% and an inner surface of more than 550 m²/g. Most of this surface is due to nanometer sized pores comparable to the situation in wood. On average, these nanopores are randomly oriented with respect to the macroscopic peel directions. The micrometer sized pores of the cell lumina exhibit a gradient from small oriented pores at the exocarp (outer part of the peel) to large non-oriented pores as well as smaller non-oriented ones in the endocarp (Fig. 3).

Fig. 3 SEM images of the gradient foam structure of a pomelo (left) and its silica replica (right).

2) X-ray scattering methods to study structure-function relations in biological materials

A long term activity of the group is the (further) development of experimental techniques based on position resolved and in-situ X-ray scattering using synchrotron radiation. They are particularly applied to relate the hierarchical structure of biologic materials to their functional properties and are performed in close collaboration with several research groups at the MPI of Colloids and Interfaces in Potsdam.

Fig. 4 Calcite and amorphous calcium carbonate in lobster cuticle.

Along similar lines, this method was used to map the Mg content in the stone part of the sea urchin tooth independently within the micrometre sized needles and plates and within the nanocrystalline matrix [3]. Several other cooperation projects dealt with structure-function relations in biological materials using X-ray techniques, such as the mechanical response on in-situ moisture changes in wood [5], the nanostructure mapping of tooth dentin [6], and zebrafish fins [7], and nanostructure of biogenic calcite in mollusc shells [8].

3) Other activities

Other activities within this group focussed particularly on the application and the further development of small-angle X-ray scattering. A cooperation project with the University of Erlangen focused on cellulose sheets as synthesis matrices of EuF₃ particles [9]. The resulting flexible sheets are transparent and show luminescence,

Recent work focused on the measurement of the local lattice spacing of biominerals in bone, crustacean cuticle, and sea-urchin teeth. Using microbeam X-ray diffraction at the μ-Spot beamline at the BESSY II storage ring in Berlin allows mapping these lattice spacings as a function of position with micrometer resolution. The shift in peak position can be related to the incorporation of substitutional elements into the crystal structure allowing to map chemical composition variations of biominerals such as Mg in calcite or Sr in hydroxyapatite [3].

Using this technique, it could be shown for instance that strontium ranelate treatment of osteoporosis results in the incorporation of Sr into the hydroxyapatite structure and not in a non-specific storage of Sr at the surface of the crystalllites. It is important to note that this result could not be obtained by standard EDX or X-ray fluorescence mapping [4]. Another investigation concerned the stabilisation of amorphous calcium carbonate (ACC) in the cuticle of lobster. One possibility that has been discussed for a long time was the possible influence of magnesium within the ACC. Upon heating, ACC transforms into calcite and microbeam diffraction allows estimating the Mg content in the original ACC phase (Figure 4). From these results, it was concluded that Mg is unlikely to be responsible for the stability of the ACC within the lobster cuticle.
making them interesting candidates for fluorescence applications. A small-angle scattering investigation of the sheets showed that they are porous with slightly oriented pores of diameters of approximately 12 nm. The EuF$_3$ particles within the sheets consist of crystallites with diameters of 10-20 nm. They form larger aggregates with sizes in the range of 200-500 nm.

**Fig. 5** Cross section Patterson functions of hexagonally arranged cylinder and inter/intra structure contributions.

The interpretation of the small angle scattering data of colloidal samples require a detailed understanding of the results expected for interacting structures [10]. Therefore we studied the Patterson functions of such structures theoretically for a range of different symmetries of the structures and relative arrangements due to the interactions (Fig. 5).

Further work was done on self assembled micelles, which are luminescent due Pt-complexes, which are not luminescent on their own [11] and on hydrotrope rich micelles and their flow behavior [12].

**Cooperation**

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**References**


Surface Physics & Scanning Probe Microscopy

Cellulose Fibers and Films

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Paper is a material made of cellulose fibers from wood, so called pulp fibers. It is not yet fully understood, how the individual fibers in paper are bonded together to form a network. In order to understand the bonding mechanisms between two fibers, atomic force microscopy (AFM) is used in two different operation modes. One AFM setup is designed to measure the fiber-fiber bond strength of two bonded pulp fibers. The other mode is imaging the cellulose fiber surface by scanning a selected area. The combination of both methods proved to be a powerful technique to gain insight into the mechanisms of fiber-fiber bond formation.

Cellulose films can be used as model systems for fiber-fiber bonds. For this purpose a comprehensive roughness characterization of the films by AFM was performed.

This work was carried out in the Christian Doppler Laboratory for "Surface Chemical and Physical Fundamentals of Paper Strength" under the coordination of Prof. Robert Schennach, Graz University of Technology.

1) Fiber-fiber bond strength

To measure the force that is needed to separate a fiber-fiber bond, the fibers are glued to a sample holder as presented in Fig. 1 [1]. The AFM cantilever is used to exert a force on the lower fiber (LF), which is only attached to the top fiber (TF) at the fiber-fiber bond. By detecting the cantilever's deflection and knowing its spring constant, the force exerted on the LF and thereby on the fiber-fiber bond can be calculated. With this setup it is possible to record the force as a function of the distance traveled by the AFM's piezo, thus force – distance curves can be plotted. One example of such a curve is illustrated in Fig. 2b.

After the breaking of the fiber-fiber bond, it is possible to investigate the formerly bonded area (FBA) with the AFM and to assign features observed on the fiber surface with force jumps in the force – distance curves. In Fig. 2c, a histogram of the force discontinuities in Fig. 2b is displayed. The force jumps can be divided into three classes (marked green, red and blue). The surface features corresponding to the force jumps are marked in Fig. 2a, where green means single microfibrils, red fibril bundles and blue cell wall delamination.

![Fig. 1 Scheme of the fiber-fiber bond strength measurement setup. TF – top fiber, LF – lower fiber, CL – cantilever, CC – cantilever chip, NP – nail polish (from [1]).](image)

2) Lignin precipitates on kraft pulp fibers

By using the AFM in tapping mode, it is possible to record – additionally to the samples topography – also a phase image. A phase image is a map of the phase shift between the exciting oscillation and the cantilever's actual oscillation. Phase mode imaging gives essentially a materials contrast. With this technique, microfibrils and lignin precipitates are revealed on a pulp fiber surface scanned in air, where the topography image yields no information about microfibrils or lignin precipitates (see Fig. 5). In Fig. 3, two phase images are depicted, the microfibrils as well as the lignin precipitates are clearly visible. Furthermore, by employing adequate analysis on the recorded phase images, it is possible to quantify the content of the lignin precipitates and their size distribution [2].
3) Cellulose fibers in water

For a deeper understanding of the bond formation between two pulp fibers, it is desirable to look at the fiber surface at a state comparable to production conditions. Since the bond formation begins with the cellulose fibers in a suspension in water, it is necessary to measure fiber surfaces in an aqueous environment. This could be achieved by employing a fluid cell and placing a droplet of distilled water on the fiber, schematically illustrated in Fig. 4.

The investigations showed that fiber surfaces in water are less wrinkled than fiber surfaces scanned in air. Furthermore, single microfibrils become visible in topography images, which are usually best visualized by phase mode imaging. AFM scans of a pulp fiber surface in air and in water are presented in Fig. 5.

Fig. 4 Scheme of AFM measurements of pulp

The roughness characterization of the cellulose films was performed in the SPM Group at the Montanuniversitaet Leoben by AFM and the strength measurements will be performed at the Institute of Solid State Physics at the Graz University of Technology.

4) Cellulose films

Cellulose films on SiO₂ were investigated as model systems for fiber-fiber bonds. The idea is to characterize the morphology of cellulose films after spin coating with xylan by roughness analysis and afterwards bonding two films together. The strength of such a bond should then depend on the roughness parameters, since the morphology defines the surface area in molecular contact. Fig. 6 illustrates how the surface morphology of a cellulose film changes after spin coating with xylan.

Fig. 6 1 μm x 1 μm AFM topography images of (a) a cellulose film on SiO₂ before spin coating; z-scale: 1 nm and (b) a cellulose film after spin coating with xylan; z-scale: 13 nm.

The roughness characterization of the cellulose films was performed in the SPM Group at the Montanuniversitaet Leoben by AFM and the strength measurements will be performed at the Institute of Solid State Physics at the Graz University of Technology.

5) Other activities

Besides investigations of cellulose fibers and films by AFM, contact angle measurements were performed on different materials. Here, surface energies of different coatings were measured in cooperation with Marisa Rebelo De Figueiredo from the Chair of Physical Metallurgy and Metallic Materials, Montanuniversitaet Leoben and Wolfgang Waldhauser from Joanneum Research, Styria.

Cooperation

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References

Surface Physics & Scanning Probe Microscopy

Electrical Characterization of Semiconductor Nanomaterials

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The increasing requirements for electronic devices inspire the development of new semiconductor materials. Novel electronic devices should be fast, energy saving, highly integrated and cheap in production. Semiconductor nanostructures like nanowires, nanorods, and nanodots are intensively investigated as building blocks for novel electronic devices. The choice of materials ranges from inorganic materials like InAs, InGaAs, ZnO etc. to organic ones like C60 or polyaniline.

For the development of such semiconductor nanostructures, nano-scale electrical characterization techniques are indispensable. Methods like conductive atomic force microscopy (C-AFM), Kelvin probe force microscopy (KPFM) and photocurrent atomic force microscopy (PC-AFM) are used for nanoscale electrical investigations of a variety of systems.

1. Inorganic Semiconductor Nanostructures

1.1 InGaP arrowhead defects

Support: FWF Project #P19636

So called arrow head defect (ADs), which are formed in heteroepitaxially grown GaInP/Ge(100) layers have been investigated by means of C-AFM and KPFM [1]. An understanding of these structures is particularly important for solar cell applications, where the ADs might act as leakage current pathways [2]. High-resolution AFM topography imaging in tapping mode revealed that the ADs have terminating planes which are composed from alternating sub-planes inclined 12° and 6° with respect to the (100) plane. These planes exhibit significantly higher conductivity compared to the surrounding matrix. Interestingly both planes, even though they appear morphologically equivalent, behave electrically different as confirmed by KPFM and C-AFM. In Fig. 1a), a topography image showing several ADs pointing to the left is depicted. The corresponding contact potential difference (CPD) map is presented in Fig. 1b). A clear CPD contrast between upper and lower terminating AD planes is visible. An additional C-AFM measurement of a single AD is shown in Figs. 1c) (topography) and d) (current map). Consistent with the KPFM results the upper plane exhibits much higher conductivity as the lower plane. The distinctive electrical behavior of the ADs might be attributed to a higher degree of ordering within the ADs.

1.2 ZnO nanorods

Support: FWF Project #P19636

We applied C-AFM and PC-AFM for the nanoscale characterization of as grown n-type ZnO nanorods (NR) [3,4,5]. ZnO is a wide band gap semiconductor (Eg=3.37 eV) with potential applications like ultra violet optoelectronic devices (solar cells, lasers, LEDs,..) or gas sensors. Due to the high surface to volume ratio of ZnO NRs surface related properties gain importance. Therefore, the characterization of individual NRs is of particular importance. Fig. 2. shows the local current-to-voltage (IV) characteristics for the top and side facet of an itilted NR grown on ITO by thermal evaporation (TE).

![Fig. 2. IV curves from the side (upper curve) and top (bottom curve) from an individual ZnO NR](image)

The IV characteristics of the side facet is much steeper than for the top facet which indicates the formation of different Schottky contacts between AFM tip and the different facet types.

The electrical behavior in the dark and under illumination was investigated by means of PC-AFM [4]. A principal scheme of the setup is depicted in Fig. 3a). A pronounced change in the IV characteristics upon
illumination with the full spectrum of a 150 W Xe lamp could be observed as depicted in Fig. 3b). Firstly, the onset voltage in forward direction (negative sample bias) was noticeably reduced. Second a significant increase of the reverse current (positive sample bias) was observed. Fig. 3c) shows the photo-response as a function of photon energy. Interestingly, the photocurrent onset is already detectable at 3.1 eV which is below band gap.

Fig. 3. a) Scheme of the PC-AFM setup for an individual ZnO NR. b) dark (green) and bright (red) IV characteristics c) Current as function of photon energy.

2 Organic semiconductors

2.1 Electrical properties of C₆₀


C₆₀ is an organic n-type material which is used as electron collector in organic solar cells. In this study, we applied Photoconductive Atomic Force Microscopy (PC-AFM) [6]. In order to investigate the temperature dependence of the photocurrent in C₆₀ thin films under different levels of illumination. The films were grown on ITO by Hot Wall Epitaxy (HWE) and measured with PC-AFM in nitrogen atmosphere to avoid degradation. The charge carrier concentration was modulated by varying the light intensity. In Figs. 4a) and b) topography and corresponding current images for a hot wall epitaxy grown C₆₀ film on ITO are shown. Interestingly, C₆₀ grains with totally insulating behavior were found adjacent to conductive ones (see Fig. 4c)). As depicted in Fig. 4d) no significant influence of the light intensity on the current was observed.

Fig. 4. a) Topography image of C₆₀/ITO grown by HWE (z-scale 50 nm). b) corresponding current (10 pA scale) c) height and current profiles along the green lines in a) and b). d) Arrhenius plot of the current densities for different light intensities.

2.2 Organic polymer blends

Support: FWF NFN projects #S9707-N20 and #P19636.

AnE-PVs:PCBM blend films for polymer solar cells have been investigated by means of C-AFM in UHV. In Fig. 5, the topography image a) and corresponding dark current image b) at 5 V sample bias are shown. Conductive areas could be identified coinciding with grains in the topography. This was interpreted as areas with higher PCBM concentration.

Fig. 5. a) Topography image of AnE-PVs:PCBM (z-scale 15 nm) and corresponding current image b)(current scale 5 nA)
2.3 UV induced modulation of the conductivity of polyaniline


The UV induced change in conductivity of polyformylaniline (PFANI) has been investigated by means of C-AFM [6]. A photodecarbonylation reaction transforms PFANI to polyaniline (PANI). UV-illumination through a mask and successive protonation results in films with a pattern of conductive and insulating areas. C-AFM images were measured for illuminated samples before and after protonation in HCl vapor. Fig 6 a) and b) represent the current image together with the corresponding line profiles prior to protonation. A slight conductivity increase is observed at the irradiated areas. As visualized in Fig 6 c) and d) the successive protonation increased the conductivity by several orders of magnitude. Therefore it is proven that PANI is suitable for the fabrication of sub-µm conductive patterns via UV illumination.

![Fig. 6. a) Current image (current scale -15 fA) of illuminated non protonated PANI b) corresponding line profiles along the black line in a). c) Current image for illuminated and protonated PANI (current scale -100 pA). d) Corresponding line profiles along the black line in c).](image)

References

Cooperation
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Organic semiconductor thin films

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In the last three decades, significant progress has been made in developing organic semiconductor molecules and applying them in so-called organic electronics. Nevertheless, the basics in thin film growth of organic molecules are not yet fully understood. Especially, knowledge of the initial nucleation process during deposition of conjugated molecules will be crucial for the design of growth routes resulting in smooth films of defined molecular orientation. Such films are a prerequisite for the fabrication of electronic devices like organic light emitting diodes (OLED), organic solar cells, and organic field effect transistors (OFET). We were investigating the growth mechanisms of the rod-like oligophenylene molecule para-hexaphenyl (6P, C_{36}H_{26}) on amorphous substrates by atomic force microscopy techniques (AFM) as well as the initial growth of the same molecule on the novel substrate graphene by low-energy electron microscopy (LEEM).

Evaluation of the critical island size in 6P islands on amorphous substrates

For the understanding of the initial mechanism of thin film growth, the critical nucleus size or critical island size \( i^* \) is very crucial. 6P was evaporated onto two different amorphous substrates (silicon dioxide and ion-sputtered mica) by using organic molecular beam epitaxy (OMBE) in ultra-high vacuum (UHV). The amorphous substrates had been chosen, because 6P builds islands (and later terraced mounds, see Figure 1c,d), molecule length: 2.6 nm) of up-right standing molecules during the nucleation process [1]. The silicon based samples were prepared here in Leoben and the mica based samples were provided by our collaborators from Graz. All samples were investigated ex-situ by AFM in tapping mode. Figure 1a) shows an example of a submonolayer of 6P on silicon dioxide. As a first step to obtain \( i^* \), the AFM image has to be overlaid by a mesh by Voronoi polygons (Voronoi tessellation, see Figure 1b). These polygons correspond with capture zones around the islands for single molecules which hit the surface during evaporation. \( i^* \) can be evaluated by different approaches. Here we used – for the first time for organic thin films – a recently developed approach based on capture-zone scaling, using the generalized Wigner surmise (GWS) [2,3]. The areas of the capture zones are presented in a histogram and then complemented by GWS functions for different \( i^* \) (Figure 2). The function which fits best with the scaled counts of the capture zones yields then \( i^* \). The results for \( i^* \) on the two substrates are different from each other for evaporation of 6P at room temperature: for silicon dioxide \( i^*=1 \) and for ion-sputtered mica \( i^*=3 \). These values were cross-checked independently by two other approaches – the island-size scaling by Amar/Family and Venables’ rate theory – and led to the same results [4,5].

Layer by layer growth of organic molecules on graphene

The novel material graphene bears the potential to be used as transparent flexible electrodes in OLEDs or organic solar cells. For this purpose, the organic molecules are desired to grow in a lying fashion.

![Fig. 1: (a) 20x20 μm² AFM image of a 6P film grown on SiO₂ at RT (z-scale of 5 nm). (b) Image masked with the calculated Voronoi polygons. (c) 1x1μm² AFM image of a single island. (d) Corresponding height profile represented by the red line in (c).From [4].](image)

![Fig. 2: Capture-zone histogram obtained from the sample grown at RT. About 2700 capture-zone areas were analyzed. Capture-zone distribution for several values of \( i^* \) are plotted for comparison. The dashed line is a least square fit to the data of the histogram. The thick line marks the selected \( i^* \). from [4].](image)
Low Energy Electron Microscopy (LEEM) and micro Low Energy Electron Diffraction (µLEED) have been employed to study in situ the initial growth of 6P on graphene. As substrate for these experiments we used Ir(111) supported graphene [6]. In contrast to the formation of terraced growth mounds composed of standing molecules [1] (see figure 1), here indeed layer-by-layer growth of lying molecules is observed. After formation of a low density layer, the full first 6P monolayer already shows a bulk like structure. Up to at least four monolayers grow in this fashion as is illustrated in Fig. 3.

The nucleation of the 6P islands occurs at wrinkles in the metal supported graphene layer. Larger islands composed of flat lying molecules detach from the original nucleation sites and move rapidly as entities across wrinkle free substrate areas [4]. Fig. 4a-c) shows this sequence in the series of LEEM images. Fig. 4d) explains the observed behaviour of the half-layer islands by edge diffusion and an isotropic sticking of the molecules the island edges.

Cooperation
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Fig. 3: a-c) Sequence of LEEM images of 6P on graphene. a) Graphene flake with Ir steps and wrinkles. Dark areas are half-layer 6P islands. (b) The islands visible in (a) have formed a closed initial layer (medium gray, marked by arrows). Now, a second, darker contrast develops on top of the initial layer. This full first monolayer (dark gray) is nearly completed. c) Complete first monolayer. (d) Proposed structure of 6P on metal supported graphene. Four layers of bulk-like 6P are deposited with their \{111\} plane parallel to the graphene substrate (light blue carbon atoms for clarity). The ad-layer covering 50% of the top surface is shown with orange carbon atoms. From [7].

References
Fig. 4: Three consecutive LEEM images (1 sec between images) showing the mobility of the initial islands (dark patches) on graphene. a) small 6P island is nucleated in the upper right corner next to a wrinkle and grows in size. When the accumulated stress reaches a critical level (b), the island elongates and detaches from the original site in order to move to a location further away from the wrinkle. d) Schematic 6P island outlining the possible diffusion paths and preferred incorporation sites. 6P molecules detach from the left and move toward the right side of the island. The side edges are formed by the terminating hydrogen atoms of 6P and possess a low sticking probability. Only the edges terminated by the long side of 6P have a high sticking probability due to the large number of hydrogen bonds that can be formed there. From [8].
Mechanical Characterization of thin films by transverse shear- and friction force microscopy

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These mechanical characterizations are based on atomic force microscopy to understand the growth mechanisms as well as to explore the corresponding growth morphologies in thin film systems. A small tip attached on a very soft cantilever is scanned perpendicular (FFM) or parallel (TSM) to the cantilever’s long axis on a surface in contact mode. The tip is bent by the interaction force between the tip and the surface. The lateral torsion of the cantilever can be detected by a laser beam on the four-quadrant photodetector.

We use FFM to detect chemically changes on photolithographically UV-patterned surfaces of photosensitive ultrathin films. Using TSM, the crystallographic domains and molecular orientation of the organic surface can be revealed.

This work is done within the Austrian Research Network “Interface controlled and functionalized organic films”, and funded by the Austrian Science Fund projects S9707.

1) Growth morphology

Cooperation FWF-Project S9704 with Prof. Michael George Ramsey, Cooperation Group: Institute of Solid State Physics in Graz University of Technology with Prof. Adolf Winkler

a) Para-hexaphenyl (6P) film growth on amorphous mica:

On the sputtermodified amorphous mica surface the 6P molecules form two-dimensional islands of standing molecules [1].

b) Epitaxially Grown Films of Lying Pentacene Molecules on Cu(110) Surfaces:

The morphology observed by atomic force microscopy shows an epitaxial alignment of pentacene crystallites, which forms the “single crystal” structure with molecules lying with their long axes parallel to the Cu (110) substrate [2].

2) Hierarchy of friction forces in patterns of photoreactive surface layers

Cooperation FWF-Project S9702 with Prof. Wolfgang Kern, Cooperation Group: Materials Center Leoben (MCL) with Dr. Thomas Klünsner.

FFM can be used to characterize the photolithographic modification of thin functional silane layers. The photopatterned surfaces were produced using a contact mask during illumination followed by the post-modification reaction. The changes in chemical reactivity of the surface can be sensitively detected by the changes of the lateral torsion of the FFM cantilever induced by surface friction force. Friction force microscopy (FFM) can reveal the contrast between modified and unmodified regions of the patterned surfaces [3]. The friction coefficients on the surface can be determined [4].
Fig. 3 Friction force microscopy (FFM) image of the thin silane layer (8 nm) with a mask (3µm lines and spaces): (A) morphology (z-scale 10 nm), (B) resulting friction contrast (z-scale 150 mV). The inset in (B) shows a 1D-FFT perpendicular to the stripes.

Fig. 4 (a) Topography of a V2O5 film grown at 230 °C on MgO(001), (b) corresponding FFM image, which determined the friction coefficient µ=0.6.

3) Molecular alignment on the surface of organic thin films

Cooperation FWF-Project S9708 with Prof. Roland Resel, Cooperation Group: Institute of Solid State Physics in Graz University of Technology with Prof. Adolf Winkler

The self-assembly of monolayers is a highly promising approach in organic electronics [5]. Using TSM, the different molecular alignment on the SAM surface can change the cantilever’s lateral torsion, which is very sensitive to the crystallographic orientation on the surface. The shape and size of the crystallites can be determined: polygonal shapes with lateral sizes of several micrometers were observed [5].

Fig. 5 (A) Topography of a monolayer SAM annealed at 400K, (B) corresponding TSM image with additionally drawn clear domain boundaries (thick lines) and proposed boundaries (dashed lines).

4) Other activities

FFM and C-AFM measurements of ion bombardment graphite samples and of tribological films

Cooperation

References
ZnO Varistor Ceramics

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Varistors are electroceramic components, used as overvoltage protection in electronic devices. The standard varistor material is polycrystalline ZnO which shows highly non-linear current-voltage characteristics with rapidly decreasing resistance above a specific voltage. This effect is caused by double Schottky barriers at the grain boundaries, symmetrical barriers at the grain boundaries are assumed.

Cross sections of ZnO varistors from EPCOS-TDK OHG Deutschlandsberg were prepared and investigated with Kelvin probe force microscopy (KPFM), conductive atomic force microscopy (C-AFM) and electron backscatter diffraction (EBSD).

KPFM
The presented KPFM and EBSD investigations were made on a praseodymium doped multilayer varistor sample. Fig. 1 shows an AFM height image (a) with the corresponding contact potential difference (CPD) image (b) from KPFM and the corresponding crystallographic orientations (c) measured with EBSD. For the measurements presented in Fig. 2, bias voltages of +1 V and –1 V, respectively, were applied between the electrodes. In the surface potential map (Fig. 2 a), the ZnO grains can be seen as equipotential areas and the voltage changes only at the grain boundaries. This means that the resistances of the grain boundaries are much higher than those of the bulk material. The difference between the electrodes and the adjacent ZnO grains is caused by the workfunction difference. The potential profiles in Fig. 2 b) and c) are taken along the lines 1 and 2 in Fig. 2 a). The profiles in Fig. 2 b) are taken with a bias of -1 V, the profiles in Fig. 2 c) are taken with a bias of +1 V applied. These cross-sections are taken in an area with only one ZnO to ZnO grain boundary between the electrodes and the grain on the right side is the same for both lines. In Fig. 2 b) with -1 V, both lines overlap also on their left grain with only a small difference caused by the difference in CPD. The cross section in Fig. Fig. 2 c) shows a clear difference in potential of the two left grains which cannot be explained by the difference in CPD. We assume that the barrier between ZnO and the electrode material becomes more pronounced because of a lower barrier at the ZnO grain boundaries along line 2. This grain boundary with a reduced resistance is causing a localized current flow and a local heating of the varistor.

Fig. 1: Investigation of a polished varistor: a) AFM height image, b) CPD image, c) EBSD map of a varistor sample

Fig. 2: a) surface potential map @ +1V, b) cross section -1V, (c) cross section +1V
C-AFM
The investigations shown in Fig. 3, were performed on a Bi$_2$O$_3$ doped multilayer varistor sample. Conductive AFM (C-AFM) measurements were performed to record the I-V characteristics of individual grains. Fig. 3 a) shows the height image with the corresponding current image in b). Individual ZnO grains and the spinel phase between the ZnO grains can be seen in the height image as well as in the current image. In the current image, the grains closer to the electrode show a higher current and the spinel phase is insulating. The scanning electron microscope (SEM) image in c) shows a larger sample surface section to illustrate the distance from the area of the AFM scan to the electrode. The sample was etched with HF after AFM and prior to SEM investigations to increase the visibility of the grains and phases in SEM images.

The I-V curves in Fig. 4 correspond to the positions 1 – 4 marked in Fig. 3 b) and were acquired from the marked rectangles averaged values from scans with different voltages applied.

Pos. 1 is on a nonconductive spinel phase. Pos. 2 is on a grain with only one ZnO grain between the measured grain and the electrode. The positions 3 and 4 are on two halves of a grain with a twin boundary and two ZnO grains to the electrode. Pos. 2 shows a significantly lower resistance compared to Pos. 3 and 4. The two measurements on the twinned grain differ slightly but significantly with a higher resistance on Pos. 4. The nonlinear behavior can be seen on all measurements on ZnO.

Fig. 4: I-V characteristics at the positions 1-4 (marked in Fig. 3).

Cooperation
This work is performed in collaboration with the Institute for Structural and Functional Ceramics and EPCOS-TDK OHG Deutschlandsberg under the FFG bridge project (824890) “Zusammenhang zwischen dem Mikrogefüge und den makroskopischen, elektrischen Eigenschaften von Zinkoxid-Varistoren”.

References
Photonics Crystals for Optoelectronics

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Photonic Crystals (PhCs) are structures with a spatially periodic dielectric constant (and refractive index). Such periodic dielectric structures show band gaps. A gap forbids propagation of a certain frequency band of light [1]. This property enables one to manipulate the light in a controlled way. The formation of the gaps can be tuned by changing e.g., the refractive index by a magnetic field applied to the PhC [2]. Therefore, PhCs are devices highly suitable for e.g. information processing, generating structural colors or the optimization of certain electric field components in optical devices.

1) Optimizations of quantum well infrared photodetectors (QWIP)

PLATON 35N (FFG)

A typical application for QWIPs is thermal imaging. QWIPs detect mid infrared radiation in photoconductivity by exciting electrons out of GaAs/GaAlAs quantum wells into the conduction band. However, this transition is sensitive to the electric field component normal to the GaAs layer. This component is small or, for normal incidence, absent. However, it can be enhanced by using PhC structures. Here, we perform simulations on the field distribution for different QWIP structures. As a simulation tool the finite difference time domain (FDTD) method is used. In particular two systems were studied: (a) A structure with a sacrificial layer [blue in Fig. 1(a)] which can be removed to form a free-standing PCS and (b), a structure with a QWIP perforated by air holes on top of a GaAs substrate covered by a metal hole array (MHA) [3] [see Fig. 1(b)].

In (a) three-dimensional finite difference time domain (FDTD) calculations of the propagation of waves in the PhC-QWIP structure were performed. The wavelength dependence of the mean field component in growth direction $<E_y^2>$ was determined. The simulation results show high agreement with the experimental results.

In addition we performed simulations for different refractive indices of the spacer below the PhC from $n_{sp}=1$ for the freestanding PhC slab (removed sacrificial layer) over $n_{sp}=2.9$ (original layer) to $n_{sp}=3.12$ (no index contrast). The simulation showed a strong response of the PhC resonances to the variation of the refractive index. A decrease of the PhC resonances by increasing the refractive index has been observed. An analysis of the modes from the $E_y$ field distribution in the $x$-$z$ plane yielded information about the shift of the resonances to lower wavenumbers with increasing refractive index. From the obtained simulations we are able to conclude clearly, that the use of free standing photonic crystal slabs for QWIPs results in strong absorption enhancement, which is essential for high signal-to-noise ratios in these devices.

In (b) it was shown that structures consisting of a metal hole array (MHA) lying on top of a 2D PhC exhibit extraordinary exhibit the extraordinary transmission effect [1]. In detail it could be demonstrated that the extraordinary transmission in such hybrid structures is due to the coupling of an incident wave to the eigenmodes of the PhC. Therefore, the peaks in the transmission are determined by the spectral position of the respective PhC eigenmodes. The results showed a novel approach to manipulate light on a subwavelength scale.

Fig. 1 Structure (a): PCS structure. the layered part symbolizes the multiple GaAs/GaAlAs quantum wells. The blue part indicates a sacrificial layer. By removing it ($n_{sp}=1$) the layer above forms a free-standing PCS. The brown layer below represents the GaAs substrate. (b) Hybrid MHA/PhC structure. The golden top layer symbolizes the MHA.

Fig. 2 Field distribution for a free standing PCS ($n_{sp}=1$) structure
Cooperation
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2) Design of polymer-based-fiber to silicon-waveguide couplers

![Fig. 3](image3.png)

Fig. 3 silicon (red) to polymer-based(green) coupler Distribution of the electrical field components for the structure.

Project PLATON SiN (FFG)
Integrated photonics silicon dielectric waveguides are used to transmit infrared signals within integrated circuits. An important task is the optimization of the coupling of infrared radiation into the silicon waveguide. Here, two concepts have been analyzed by using three-dimensional FDTD calculations: (a) the tapered waveguide coupler and (b) a coupler based on short range surface plasmon polaritons (SRSPP).

The tapered waveguide under investigation in (a) consists of three main components: a polyamide waveguide, an inversely (widening) tapered silicon waveguide and the SiO2 substrate. The individual components are defined by their dimensions and refractive indices. The source is defined by a monochromatic plane wave which irradiates into the polymer waveguide. In detail, the influence of the height of the Si waveguide and the length of the polyamide waveguide on the coupling have been investigated. First results showed that an optimal length of the polyamide-waveguide exists. Further simulations showed that the coupling efficiency increases by increasing the height of the Si waveguide.

In concept (b), in addition to the dielectric waveguide made of Si, in order to efficiently transfer radiation into the dielectric waveguide an intermediate plasmonic wave guide made from a thin metallic strip-line has been implemented [4]. By using a thin metallic strip-line the plasmonic waves penetrate the metal layer. Coupling between a short range plasmon polariton (SRSPP) mode and the dielectric waveguide mode can be achieved. This coupling is studied by using the FDTD method. As cladding a SiO2 matrix is assumed. The task was to optimize the dimensions for the Si waveguide to achieve best possible coupling.

Fig. 4 Silicon-metal-polymer coupler structure.

Cooperation
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3) Other activities: Wave propagation in disordered solids – heterogeneous rocks

The propagation of electromagnetic radiation, in particular microwaves, in rocks is of great interest for a reduction of the energy consumption during the fragmentation of rocks, e.g. for tunnelling, extraction of valuable ores, and processing of pre-conditioned rocks, see e.g. Ref [5]. The required amount of energy is of the order of several percent of the total energy consumption worldwide. Only less than 1 % of this energy is actually used for the generation of new surfaces. Many of the techniques applied use mechanical cutting tools. Techniques assisting these tools have a high potential for reducing the energy consumption. One of them is the application of high-power microwaves prior to the mechanical treatment. The purpose is to heat the rock in a way that large temperature gradients are established that lead to thermally induced stresses which should exceed the strength of the material and lead to the generation of cracks.
In our studies (Fig. 5) we consider a block of rock with different constituents. The rock is irradiated by a microwave beam from the open end of a waveguide. From the intensity distribution in the beam the time dependence of the temperature and the stresses has to be calculated to find out at which energy input the strength of the material is exceeded. In a homogeneous material the shape of the beam is determined by Gaussian broadening. In a heterogeneous material like a rock the radiation is scattered and the beam can be broadened to a larger extent than in the Gaussian case. As a first approach in our FDTD model calculations we consider a disordered solid [7]. Here, a two-dimensional model with circular discs distributed randomly in a matrix is used. The model used, corresponds to a simplified two-component rock. The discs and the matrix are assumed to have different dielectric properties. This way the deviation from the ideal behaviour of a photonic crystal could be calculated. This enables us to calculate the field and intensity distribution of the microwave. The microwave frequency considered is in the range of 2.54 GHz, a common industrial frequency.

We conclude that only for strong differences in the dielectric properties the deviations from the Gaussian broadening will be significant. It is not expected that this conclusion will be essentially different if a multi-component rock and a three-dimensional model is considered. In future work it is planned to consider these more complex cases and to calculate the development of the stresses in cooperation with Institute of Mechanics, Montanuniversitaet Leoben.

Cooperation

References
Electron Transport Properties in Quantum Dots

Roland Brunner, Ronald Meisels, Friedemar Kuchar
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Electronic transport in semiconductor nanostructures is a key issue in condensed matter physics and nonlinear science. Important classes of nanostructures are metal-gate defined quantum dots. In these systems, electrons are restricted to a plane, the two dimensional electron gas (2DEG), near the interface between two different semiconductors. Applying voltages to contact gates deposited above the junction allows confining the electrons in submicron-sized 2D cavities. In general, the connection to the external world is through quantum point contacts (QPC). In each of these QPCs, the local potential is a saddle shape potential. If the peak of this potential is larger than the corresponding Fermi energy, then the barrier is a tunneling barrier, and the electrons within the dot are strongly quantized. Such dots can be referred to as closed dots. They are highly interesting in terms of single electron spin manipulation. Therefore, applications for quantum information processing are expected. However when the peak potential is smaller than the corresponding Fermi energy, then the transport is characterized by the formation of several conducting channels through the QPC. Due to the strong coupling to the environment, those dots are referred to as open quantum dots. Open quantum dots provide a natural system in which to study both the classical and the quantum features of transport.

1) Classical to quantum mechanical transition in open quantum dots

The understanding of the border between the classical and quantum mechanical world is highly relevant since the advent of quantum mechanics. According to [1] in an open system, the environment imposes so-called superselection rules by preserving part of the information that resides in the classical correlations between the system and the measuring apparatus, leading to an environment-induced process of superselection (einselection). This means that essentially preferred states, termed pointer states survive the decoherence process related to the coupling with the environment. Pointer states are effectively classical.

Here, we investigate the manner in which these classical states evolve into the set of quantum states (Fig. 1). Therefore, we perform classical calculations of the electrons within the open quantum dots and compare the results with quantum mechanical calculations and scanning gate microscopy experiments performed by R. Akis and N. Aoki respectively. The open quantum dots provide a mixed phase space. That is, chaotic as well as regular regions within the phase space are present. The regular regions found within the mixed phase space correspond in single open quantum dots to Kolmogorov-Arnold-Moser (KAM) islands. [2]

The trajectories that are found within the chaotic sea correspond to classically closed trajectories. Beside the single dot closed orbits another type of closed orbit arises by coupling two or more open quantum dots. This type of orbit exists on an island of attractors located within the mixed phase space [24, 25].

The combination of classical and quantum mechanical simulations showed that the closed orbits within the mixed phase space can be associated with the pointer states. Quantum states within the open quantum dots structures that couple well to the outside environment, through the QPC’s confining constrictions, are heavily decohered according to [1]. These states give rise to the chaotic sea that exists in the classical phase space of the dot.

Scanning gate microscopy (SGM) –technique in combination with transport experiments provides a powerful tool to image the motion of the electron in a quantum system, e.g. [3]. Recently we have reported on the direct imaging of specific features from single scarred wavefunctions and classical trajectories in open quantum dots. The direct imaging of such wavefunctions is important since it gives novel information about wavefunction scarring, the classical transition and dissipation in quantum systems. In addition further evidence of the emergence of the so called pointer states has been found experimentally by using SGM.

Fig. 1 Classical (white line), quantum mechanical (white contour plot, bright: high probability density, dark: low probability density) and experimental SGM results (dark: low change in the conductance, bright: large change in the conductance) superimposed on each other for different magnetic field (B) values. (a) B=0 T, (b) B=100 T, (c) B=180 T, (d) B=240 T [4].

2) Electron spin based quantum information processing with quantum dots

The bit is a fundamental concept of classical computation and information processing. A classical bit can be 0 or 1, like the tail or the head of a coin. The information flow is sequential and is able to go only in one direction. The situation is different for quantum information processing. In quantum information processing the smallest logical unit is the quantum bit or qubit. A qubit can be represented by |0> and |1> which

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give the computational basis states. The basis is orthogonal, therefore linear combination or the superposition is allowed between the two states. In addition qubits can be entangled. A change of one of the two physically separated qubits, has the same effect on the other one. Therefore, high calculation capability is obtained. In contrast to classical information processing various operations can be performed simultaneously. The spin, with $|\uparrow\rangle$ and $|\downarrow\rangle$ and all linear combinations, is predicted to be a good candidate for qubits [5]. It forms a natural two level system. Advances in semiconductor quantum dot technology have enabled us to detect and coherently manipulate the single electron spin, e.g. [6,7]. However, for quantum computation the one-qubit operation is not sufficient. In addition an entangling two-qubit operation is necessary. It was demonstrated that an entangling two-qubit operation can be achieved by using a double quantum dot with a split micro-magnet design. With this approach it is possible to create a sequence of various quantum operations, including specific single spin rotations and a two-qubit exchange operation in the inhomogeneous magnetic field produced by the micro-magnets (Fig. 2). The results are highly important to achieve the universal set of quantum operations necessary for quantum computation. 

**Fig. 2** Schematic showing the cycle of the two-qubit operation with source (S), drain (D), $\varepsilon$ corresponds to the detuning between the two dots, left (L), and right (R) QDs.

**Cooperation**

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**References**

Numerical Simulation of Transport in Electronic Systems

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1) Numerical Simulation of Scanning Gate Experiments in the Quantum Hall Effect Regime

In addition to the search for suitable host systems and appropriate components for quantum coherent devices, also the understanding and modelling of transport in coherent electron systems needs to be improved. For this purpose the quantum Hall (QH) regime remains a major challenge, because it allows studying coherent quantum transport on a very fundamental level. In combination with the scanning gate microscope (SGM), the QH system may allow further understanding of transport in coherent systems. A gate tip introduces a local distortion and the response of the device is recorded versus tip position. In contrast to other scanning probe methods SGM does not destroy coherence and can therefore be used to investigate coherent transport. However, due to the lateral extension of the tip potential the observed responsivity maps cannot be always interpreted simply as real space images of the involved quantum states, because the observed patterns may result also from complex interactions in the tip region. Therefore numerical simulations are needed to support interpretation of SGM images. We use our non-equilibrium network model (NNM) for transport [1] and combine it with a fully quantum mechanical many particle calculation of the disordered electron system on the Hartree-Fock (HF) level (applying the code of the authors of Ref.2 with adaptations for using with the NNM).

It is well known, that in mesoscopic QH systems the plateau transitions are accompanied by magneto resistance fluctuations due to quantum coherence of the involved electronic states. The disordered potential of the electronic system can be understood as a native random arrangement of quantum dots and quantum point contacts, which interact in a complex way. Either caused by a sweeping magnetic field or by moving a biased gate tip, any changes of the quantum states are sensitively monitored also by the Hartree part of the self consistent Hartree-Fock solution, which modulates the transmission behaviour of the involved saddle potentials. That is sensitively detected by our network model and results e.g. in resistance fluctuations. Some simulation results for both, magneto resistance fluctuations and responsivity maps for a moving gate tip are presented in Fig. 1-3. The importance of the electron-electron interaction in our simulations is demonstrated by turning on and off the Hartree part of the Hartree-Fock solution for the screened random potential.

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Some results for magneto resistance and scanning gate simulations

![Simulation result for the total sample conductance as a function of the magnetic field at fixed gate tip position, in red for a full HF calculation and in black the calculation without the Hartree part of the Hartree-Fock (HF) solution.](image1)

![Simulation result for the total sample conductance as a function of the magnetic field at fixed gate tip position, in red for a full HF calculation and in black the calculation without the Hartree part of the Hartree-Fock (HF) solution.](image2)
Fig. 2: Simulation result for longitudinal (top) and Hall resistance (bottom) with (red) and without (black) Hartree-part of the HF solution.

Fig. 3 Map of total conductance in units of $e^2/h$ as a function of tip position, the scanning tip potential amplitude $V_{\text{tip}}$ was set to 5mV. Top: result by using full HF solution and bottom: result without Hartree part of the HF solution.

2) Numerical Studies of Non-local Magneto Transport Effects in Quantum Hall Device Structures

There are an increasing number of devices applying quantum Hall systems for various purposes. One is spintronics in context with injection and detection of spin polarized electrons, but there are also other device concepts like electron interferometers or terahertz emitters [1], which make use of the unique properties of edge states. Besides the clear and well defined device concepts there show up lots of “side effects” in real experiments, which make it difficult to interpret experimental results in all details. This difficulty results mainly from the fact that in general one has to deal with a certain degree of in-homogeneity of the electronic system while the sample geometry gets more complicated at the same time. This makes it difficult to sort out pure geometry and contact effects from the experimental data. Another most important aspect is that most of the theoretical approaches rely on the equilibrium situation, while an experimental investigation always drives the system out of equilibrium so that in real experiments one measures non-equilibrium currents and potentials. An appropriate model should therefore cover all these aspects and has to provide a link between the microscopic physics and the experimental answer of the complex and finally macroscopic sample.

We developed a non-equilibrium network model for magneto transport in 2D electronic systems in the quantum Hall effect regime, which is able to capture the real sample geometry, including contacts, leads and in-homogeneities like introduced by gate electrodes. The intention of our network approach to magneto transport is to address directly the non-equilibrium current flow. This means that we have to deal with the situation of a non-uniform lateral distribution of the chemical potentials. We use a network of directed quantum channels, which interconnect a two-dimensional arrangement of nodes. The directed channels keep their chemical potentials between the nodes, while the nodes transmit and modify the chemical potentials from the incoming to the outgoing channels [2,3]. It has been demonstrated, that most complex sample geometries, including gate effects and the effect of non-ideal contacts can be successfully described by our network model [see e.g. 4,5,6,7].

We investigated non-local effects in magneto transport for a number of contact configurations of a quantum Hall system, including the effect of having unused metallic contacts between the active region of classical current flow and the remote region where the non-local signals are obtained. Just to mention one of the examples, we divide a Hall bar in longitudinal direction into two parts by applying an additional current contact at about half length of the sample. Even if we now restrict the classical current flow to one of the two parts of the Hall bar only, we can still get a non-local signal between the remote Hall voltage probes in the classically current-less remote part of the Hall bar. This is demonstrated to occur, if the additional current contact does not act as an ideal contact for the edge channels.

References
3) Numerical Studies of Magneto Transport in 2D Electronic Systems in the Presence of Non-Uniform Magnetic Fields

Non-uniform magnetic fields play an increasing role in device concepts during the last decade [1,2]. One key point is that magnetic field gradients create barriers [see e.g. 3], which act in addition to eventually present electric barriers. While theoretical approaches mostly rely on the equilibrium situation, experiments drive the system out of equilibrium so that in real experiments one always measures non-equilibrium currents and potentials. An appropriate transport model should take care of this and has also to provide a link between the microscopic physics and the experimental answer of the finally macroscopic sample. We developed a non-equilibrium network model for magneto transport in 2D electronic systems in the quantum Hall effect regime, which is able to capture the real sample geometry, including contacts, leads and in-homogeneities like introduced by gate electrodes [4-8]. This is the first time that we apply this network model also to the situation of non-uniform magnetic fields.

We restrict our considerations to two basic configurations for a standard Hall bar structure: (i) a hybrid magnetic-electric confinement at the edge and (ii) a magnetic barrier located in the bulk, which is aligned in longitudinal and transverse direction.

FIGURE 4 Different non-uniform magnetic field distributions as used for the simulations. For the hybrid confinement we use a parabolic function of B versus distance from the sample center (dashed line) and constant field in longitudinal direction. For the magnetic barrier we use a Gaussian function in one direction and constant field in the other direction (thin solid line), which in this figure corresponds the longitudinal orientation. The selected carrier density is 4x10^11 cm^-2 and the Hall bar is mapped onto a 120x60 network grid.

Fig. 4 shows the applied magnetic field distribution, which is superimposed on the main uniform sweeping magnetic field of the Hall experiment. Fig.5. shows simulation results for R_{xx} of the \nu = 4 \rightarrow 3 plateau transition for all different cases of the non-uniform field. For the hybrid magnetic - electric confinement one can clearly see, that R_{xx} gets more and more suppressed with increasing field gradient at the edge. This can be understood in terms of a suppression of edge bulk equilibration because of the additional magnetic field gradient. The magnetic field gradient near the edge creates compressible and incompressible stripes also away from the real sample edge. This acts like a softening of the real edge potential, which reduces equilibration. Therefore less dissipation occurs, which is responsible for the R_{xx} peak height. This reduces also the coupling between contacts and inner edge channels, which leads to a more complex lateral potential distribution and a slight shift of the R_{xx} peaks (details will be published elsewhere). R_{xy} (not shown) does not show significant features.

FIGURE 5 Results for R_{xx} of the \nu = 4 \rightarrow 3 plateau transition for hybrid confinement at different non-uniform field strength (dashed lines) and for a magnetic barrier of fixed shape but for longitudinal and transverse orientation (thin solid lines). The bold line represents R_{xx} for uniform field. B_{conf} represents the used value of the superimposed non-uniform field at the sample edges.

Looking at the effect of a magnetic barrier, which was chosen with fixed shape and height (Bz=0.3T), we can clearly see, that the parallel orientation of the barrier reduces R_{xx} as compared to the situation of a uniform magnetic field, while the transverse orientation of the barrier increases R_{xx}. Since the transverse orientation of the magnetic barrier creates a real barrier for the longitudinal current flow, the longitudinal orientation creates a barrier for the back scattering process, which is indicated by the reduction of R_{xx}.

Acknowledgments

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27. Todt, M.; Rammerstorfer, F.; Paris, O.; Fischer, F.D., Nanomechanical Studies of the Compressive
28. Zabler, S.; Paris, O.; Burgert, I.; Fratzl, P., Moisture changes in the plant cell wall force cellulose
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Book contributions 2010/2011

**Other publications 2010/2011**


**5. Presentations**

**Talks at conferences 2010**

2. Beinik, I.; Kratzer, M.; Teichert, C.; Galiana, B.; Rey-Stolle, I.; Algora, C.; Tejedor, P. *Nanoscale electrical characterization of arrowhead defects in GaInP thin films grown on Ge*. 37th Conference on the Physics and Chemistry of Surfaces and Interfaces. Santa Fe, New Mexico, 10.01.2010
6. Erko, M.; Findenegg, G. H.; Cade, N.; Michette, A. G.; and Paris, O.; *Raman scattering on confined water*. CONFIT 2010 - Dynamics in confinement. ILL, Grenoble, 03.03.2010


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37. Teichert, C. (Invited) Quantitative surface characterization by atomic-force microscopy. 4th Intl. SAXS/GISAXS Workshop., 09.09.2010


40. Teichert, C. (Invited) Thin Film Characterization by Transverse Shear Microscopy and Photoconductive AFM. Seminar within AFM Workshop at University of Linz. JKU Linz, 25.11.2010

41. Teichert, C. Die Zukunft der Halbleiterwerkstoffe: Werkstoffcharakterisierung auf der Nanoskala. Veranstaltung Nr. 160.LW17 Werkstoffe der Zukunft., 29.01.2010

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47. Weber, A.; Resch, K.; Teichert, C. Atomic force microscopy as metrology tool for identification of phases in two- or multi-component polymer systems. 10th Austrian Polymer Meeting and 2nd Joint Austrian-Slovenian Polymer Meeting. Leoben, 08.09.2010


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30. Schmied, F.; Fischer, W.; Hirn, U.; Schennach, R.; Teichert, C. Mechanical properties of fiber-fiber bonds in paper studied by atomic force microscopy. 75. Annual Meeting of the DPG and combined DPG Spring Meeting. Dresden, 13.03.2011


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Invited talks at external institutions: Seminars 2010/2011

4. Oswald, J. Introduction to the quantum Hall effect. Gastvortrag/Seminar. Chiba University, 23.06.2011
5. Oswald, J. The role of non-homogeneities and contacts in quantum Hall. Gastvortrag/Seminar. Chiba University, 01.11.2011
20. Teichert, C. Electrical characterization of semiconductor nanostructures. Seminar, Department of Physics, Hong Kong University. Hong Kong, 11.01.2010
23. Teichert, C. Nanostructure characterization utilizing Scanning Probe Microscopy. Seminar, School of Materials Science and Engineering, East Chinese University of Science and Technology (ECUST), Shanghai. Shanghai, 30.08.2010
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11. Erko, M. Small-Angle x-ray scattering on confined water. COST Action MP0601 Meeting Short Wavelength Laboratory Sources. Southampton, United Kingdom, 18.11.2010


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6. Research Projects

§ 26 – Projects

Project: “The role of interfaces for reversible and irreversible deformation of biological materials”
Funded by: FWF (P22983-N20)
Start: 1 Sep 2011
Duration: until 31 Aug 2014
Applicant: M. Hartmann
Agent: S. Nabavi
Funding: € 141,000,--

Project: “Exploring fundamental growth morphologies in organic thin film systems”
Framework National Research Network “Interface controlled and functionalized organic films”
Funded by: FWF (S9707-N20)
Start: 1 Feb 2009
Duration: until 31 Jan 2012
Applicant: C. Teichert
Agent: G. Hlawacek, St. Lorbek, Q. Shen, A. Pavitschitz
Funding: € 250,000,--

Project: “Circuit type simulations of the quantum electron transport”
Funded by: FWF (P18942-N20)
Start: 6 Nov 2006
Duration: until 6 Nov 2011
Applicant: J. Oswald
Agent: Ch. Uiberacker
Funding: € 207,000,--

Project: “Electrical properties of thin films on the nanometer scale”
Funded by: FWF (P19636-N20)
Start: 1 Jun 2007
Duration: until 31 Mar 2011
Applicant: C. Teichert / A. Andreev
Agent: I. Beinik, M. Kratzer
Funding: € 162,000,--

Project: “Hierarchically structured porous ceramics and composites from nanocasting of Plant cell walls”
DFG Framework: Biomimetic Materials Research: Functionality by Hierarchical Structuring of Materials (SPP 1420), Period 1
Funded by: DFG (Project Number 566678)
Start: 1 Dec 2009
Duration: until 30 Nov 2011
Applicant: O. Paris
Agent: G. Popovski
Funding: € 145,000,--

Project: “Ferromagnetic Semiconductor Hetero- and Nanostructures based on GeMnTe grown by Molecular Beam Epitaxy”
Funded by: FWF (P18942-N20)
Start: 1 Dec 2009
Duration: 31 Jan 2011
Applicant: R.T. Lechner
Agent: R.T. Lechner
Funding: 287.000,--

§ 27 - Projects

Project: “Hierarchically structured porous ceramics and composites from nanocasting of Plant cell walls”
Funded by DFG Framework: Biomimetic Materials Research: Functionality by Hierarchical Structuring of Materials (SPP 1420), Period 2
DFG (Project Number 587998)
Start 1 Dec 2011
Duration until 30 Nov 2013
Applicant O. Paris
Agent G. Popovski
Funding: € 165.000,--

Project: “Zusammenhang zwischen dem Mikrogefüge und den makroskopischen, elektrischen Eigenschaften von Zinkoxid-Varistoren”
Funded by: FFG BRIDGE-Brückenschlagprogramm (824890)
Start: 1 Mar 2010
Duration: Until 28 Feb 2013
Coordinator: Christian Teichert
Agent: M. Kratzer, A. Pavitschitz
Funding: € 150.000,--

Project: PLATON II
PLATON - SiN - Silicon nanostructures for photonics
PLATON-35N - III-V Nanophotonics
Funded by: FFG Österreichische NANO Initiative (1100)
Start: 1 Mar 2009
Duration: until 28 Feb 2012
Coordinator: R. Meisels
Agent: O. Glushko, R. Brunner
Funding: € 200.286,--

Other Projects

Project: CD Labor Papierfestigkeit
Funded by: Christian Doppler Gesellschaft
Start: 1. Jan 2007
Project leader: R. Schennach, TU Graz
Co-Project leader C. Teichert
Agent: F. Schmid
Funding: € 300.000,--

Project: “Growth of magnetic nano-objects by self-organization on various templates”
Funded by: ÖAD/ Wissenschaftlich-Technisches Abkommen mit Frankreich, Amadee 2009-10 (FR 13/2009)
Start: 1 Jan 2009
Duration: until 31 Dec 2010
Applicant: C. Teichert
Co-Applicant: L. Masson, Institut CINAM.CNRS, Marseille France
Agent: I. Beinik, M. Kratzer, Q. Shen, Ch. Hofer
Funding: € 6000,--

Project: “Formation mechanisms and quantum effects in Ge quantum dots on Si(001) and Si(111)”
Funded by: ÖAD/ Wissenschaftlich-Technisches Abkommen mit der Ukraine (UA 11/2009
Start: 1 Jan 2009
Duration: until 31 Dec 2010
Applicant: C. Teichert
Co-Applicant: A. Naumovets, Insitute of Physcs of National Academy of Sciences of Ukraine, Kiev, Ukraine
Agent: I. Beinik, St. Lorbek, M. Kratzer, Q. Shen.
Funding: € 6000,--

Project: COST Action MP0601
Short wavelength laboratory sources
Funded by: EU
Start: 19. May 2009
Duration: 1 Oct 2011
Project leader: O. Paris
Agent: M. Erko
Scope: Development of an in-situ Gas-sorption apparatus in connection with a laboratory based Small-angle X-ray scattering system

7. Diploma and Doctoral Theses

7.1 Diploma Theses

Mario LUGGER
Supervisor: C. Teichert
Since: Apr 2011
Friction reduction between polymer and injection mold surface: Influence of surface roughness on surface energy and interfacial tension

Lin WANG
Supervisor: C. Teichert
M. Kratzer
Since: Jan 2010
Conductivity investigation on ZnO nanorods using atomic-force microscopy

Christian GANSER
Supervisor: C. Teichert
Finished: Jun 2011
Surface characterization of cellulose fibres by atomic force microscopy in liquid media and under ambient conditions

Abdellatif JERRAR
Supervisor: C. Teichert
Finished: Sep 2011
Atomic force microscopy based characterization of photoreactive polymerthinfilms

Astrid WACHAUER
Supervisor: C. Teichert
Finished: Jun 2011
Photoconductive Atomic Force Microscopy and Kelvin Probe Force Microscopy Measurements of Organic Semiconductor Nanostructures

Nurdogan GÜRKAN
Supervisor: C. Teichert
Finished: Dec 2010
Gleitstufenuntersuchungen an austenitischen Stahlproben mittels Rasterkraftmikroskopie

Andreas PAVITSCHITZ
Supervisor: C. Teichert
Finished: Dec 2010
Conductive Atomic Force Microscopy Investigations of Organic Thin Films
### 7.2 Doctoral Theses

<table>
<thead>
<tr>
<th>Name</th>
<th>Title</th>
<th>Supervisor(s)</th>
<th>Since</th>
</tr>
</thead>
<tbody>
<tr>
<td>Seyedsoran NABAVI</td>
<td>Understanding Interfaces in Biological Tissue</td>
<td>O. Paris, M. Hartmann</td>
<td>Oct 2011</td>
</tr>
<tr>
<td>Andreas PAVITSCHITZ</td>
<td>AFM based electrical characterization of ZnO based electroceramics</td>
<td>C. Teichert</td>
<td>Dec 2010</td>
</tr>
<tr>
<td>Christian GANSER</td>
<td>Investigation of mechanical and electrical Properties of cellulose fibres on the nanometer scale</td>
<td>C. Teichert</td>
<td>Oct 2011</td>
</tr>
<tr>
<td>Quan SHEN</td>
<td>Atomic-force microscopy based characterization on functionalized organic thin films</td>
<td>C. Teichert</td>
<td>Jun 2009</td>
</tr>
<tr>
<td>Stefan LORBEK</td>
<td>Molecular processes in organic thin film growth</td>
<td>C. Teichert</td>
<td>Jan 2009</td>
</tr>
<tr>
<td>Maxim ERKO</td>
<td>Water properties in confined geometry</td>
<td>O. Paris</td>
<td>Feb 2009</td>
</tr>
<tr>
<td>Franz SCHMIED</td>
<td>Atomic Force Microscopy investigations of ber-ber bonds in paper</td>
<td>C. Teichert</td>
<td>Apr 2011</td>
</tr>
<tr>
<td>Oleksandr GLUSHKO</td>
<td>Investigations of disorder in photonic structures</td>
<td>R. Meisels, F. Kuchar</td>
<td>Jan 2011</td>
</tr>
<tr>
<td>Igor BEINIK</td>
<td>Nanoscale electrical properties of phase-seperated low-conductive thin films</td>
<td>C. Teichert</td>
<td>Apr 2011</td>
</tr>
</tbody>
</table>

### 8. Incomings: Invited Guests (Seminar)

**2010**

*Thu, 16. December 2010*

**Kolloquium zu den Nobelpreisen für Physik und Chemie 2010**

Prof. Dr. Rolf Breinbauer, Prof. Dr. Christian Slugovc  
(Institut für Organische Chemie und Institut für Chemische Technologie von Materialien, Technische Universität Graz)

„Metalle verknüpfen Kohlenstoff“

Der Chemie-Nobelpreis 2010 geht zu gleichen Teilen an den US-Forscher Richard Heck und die beiden japanischen Forscher Ei-ichi Negishi und Akira Suzuki für die Erfindung einer extrem effizienten Methode zur Verknüpfung von Kohlenstoffatomen zu komplexen Molekülen. Prof. Dr. Thomas Michely  
(II. Physikalisches Institut, Universität zu Köln, Deutschland)

„Flachland: Die Welt des Graphen“

Der Nobelpreis für Physik 2010 geht je zur Hälfte an die an der Universität

Tue, 14. December 2010
Heinz Krenn (Institut für Physik, Universität Graz)
*Magnetometry on nanoparticles – from supermagnets to ferrofluids*

Mon, 13. December 2010
Jörg Neugebauer (zusammen mit SIMNET) (Max-Planck-Institut für Eisenforschung, Düsseldorf)
*Ab initio based multiscale modeling of advanced electronic, structural and biological materials*

Tue, 7. December 2010
Ulrike Diebold (Institut für Angewandte Physik, Institut für Angewandte Physik, TU Wien)
*Organic Molecules on Oxide surfaces*

Tue, 30. November 2010
Oleksandr Glushko (Institut für Physik, Montanuniversität Leoben)
*Extraordinary optical transmission and resonant polarization conversion in photonic crystal slabs covered with metal*

Tue, 23. November 2010
Christoph Dellago (Fakultät für Physik, Universität Wien)
*Nucleation in small systems: pressure induced phase transformations in nanocrystals*

Thu, 18. November 2010
Reinhold Koch (Institut für Festkörperphysik, Universität Linz)
*Interdiffusion in Heusler film epitaxy on GaAs(001)*

Tue, 9. November 2010
Igor Beinik (Institut für Physik, Montanuniversität Leoben)
*Electrical characterization of semiconductor nanostructures by Conductive- AFM and related techniques*

Tue, 12. October 2010
Heinz Amenitsch (Institut für Biophysik und Nanosystemforschung, außenstelle am synchrotron ELETTRA, Triest, Österreichische Akademie der Wissenschaften OAW)
*SAXS and other games at the Austrian Beamline @ ELETTRA*

Thu, 12. August 2010
Johannes Prass, (Department of Biomaterials, Max Planck Institute of Colloids and Interfaces, Potsdam, Germany)
*Analysis of sorption strains in ordered mesoporous materials by in-situ x-ray diffraction*

Thu, 24. June 2010
Roland Brunner, (ICORP-JST, Quantum Spin Information Project, Japan Institut für Physik, Montanuniversität Leoben)
*Towards Quantum Computation with Semiconductor Quantum Dots*

Tue, 15. June 2010
Dieter Vollath, (NanoConsulting, Stutensee, Deutschland)
*Fluktuationen bei Phasenumwandlungen von Nanoteilchen*

Thu, 6. May 2010
Alexei Erko, (Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Elektronenspeicherring BESSY II, Berlin)
*Parallel X-ray FS-Spectrometry*

Thu, 29. April 2010
Sabine Hild, (Johannes Kepler Universität Linz, Institute of Polymer Science)
*Characterization of material properties on the subµm scale using Scanning Force Microscopy*

Wed, 17. February 2010
Wolfgang Heiß, (Abteilung für Festkörperphysik, Universität Linz)
*Colloidal nanocrystals for electronic applications*
Tue, 12. January 2010 Patrick Huber, (Physics and Mechatronics Engineering, Saarland University, Saarbrücken)
“Molecular assemblies confined in mesopores: Phase transformations and transport phenomena”

2011

Thu, 15. December 2011
Kolloquium zu den Nobelpreisen für Physik und Chemie 2011
Univ.Prof. Dr. Sabine Schindler
(Institut für Astro- und Teilchenphysik, Universität Innsbruck)
„Die Expansion des Universums“
Univ.Prof. Dr. Jürgen Hafner
(Computergestützte Materialphysik, Universität Wien)
„Quasikristalle - Nobel-Preis für Chemie 2011“
Der Chemie-Nobelpreis 2011 geht an Daniel „Dan“ Shechtman (Technion – Israel Institute of Technology, Haifa, Israel) für die Entdeckung der Quasikristalle. Quasikristalle sind geordnete Festkörper mit einer "nicht-kristallographischen" Rotationssymmetrie und quasi-(fast-)periodischer Translationsordnung.

Tue, 6. December 2011 Borislav Vasic (Institute of Physics Belgrade, Serbia)
“Controlling electromagnetic fields by photonic and plasmonic crystals in the metamaterial regime”

Tue, 22. November 2011 Stanislav N. Gorb (Department of Functional Morphology and Biomechanics Zoological Institute at the University of Kiel, Germany)
"Biological Principles and Biomimetics: Adhesion and Interlocking in the Animal Kingdom"

Tue, 15. November 2011 Antonin Fejfar (Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, 162 53 Prague 6, Czech Republic)
“Microscopic Characterization of Nanostructured Silicon Thin Films for Solar Cells”

“Nanoscopy”

Thu, 27. October 2011 Stefan Kooij (Physics of Interfaces and Nanomaterials, MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands)
“Directional wetting on chemically patterned substrates”

Mon, 5. September 2011 Nobuyuki AOKI (Division of Nanoscience Graduate School of Advanced Integration Science Chiba University, Japan)
“Scanning gate imaging of semiconductor nano-structures”

Wed, 13. July 2011 Aliaksei Vetushka (Institute of Physics, Academy of Sciences of the Czech Republic Cukrovarnická 10, 162 53 Prague 6, Czech Republic)
“Mechanical and electrical properties of microcrystalline silicon thin films”

“Reliable structure to property relations in organic semiconductors”
Tue, 21. June 2011  Roman Gansch (Center for Micro and Nanostructures, TU Wien)  
"Resonantly enhanced absorption in photonic crystal slab quantum well infrared photodetectors"

Tue, 7. June 2011  Richard Weinkamer (Max Planck Institute of Colloids and Interfaces  Department of Biomaterials, Potsdam, Germany)  
"Structural adaptation and healing of bone - computer simulations on different length scales"

Tue, 24. May 2011  Peter Hosemann (Department of Nuclear Engineering, University of California Berkeley, Berkeley, CA, U.S.A.)  
"Materials in nuclear environments"

Tue, 17. May 2011  Balder Ortner (Leoben)  
The matrix method - an overdue paradigm shift in x-ray and neutron stress measurement

Fri, 13. May 2011  Aleksandra B. Djurišić (CYM, Department of Physics, The University of Hong Kong)  
"Semiconductor nanomaterials: growth, optical properties and applications"

Tue, 10. May 2011  Helga Lichtenegger (Institute of Physics and Materials Science, Department of Materials Sciences and Process Engineering, BOKU - University of Natural Resources and Life Sciences, Wien)  
"Direct writing of optical waveguides into organically modified mesoporous silica by two-photon-induced polymerization"

Thu, 24. March 2011  Karsten Hannewald (Friedrich-Schiller-Universität, Jena)  
"Polaron Transport in Organic Crystals: Theory and Modelling"

Tue, 22. March 2011  Stephan Kümmel (Universität Bayreuth)  
"Interpreting photoelectron spectra based on DFT - new hope or just hopeless?"

Tue, 2. March 2011  Yossi Rosenwaks (Department of Electrical Engineering - Physical Electronics, School of Electrical Engineering, Faculty of Engineering, Tel Aviv University)  
"Nanoscale Potential Measurements in Pentacene Thin Film Transistors and of Dopant Distribution in Silicon Nanowires"

Wed, 23. February 2011  Franz J. Schmied (Institut für Physik)  
"What bonds paper together?"

Tue, 1. February 2011  Roland Würschum (Technische Universität Graz, Institut für Materialphysik)  
"Nanocrystalline and nanoporous materials: Atomic defects and tunable properties"

Tue, 25. January 2011  Friedemar Kuchar (Institut für Physik, Montanuniversität Leoben)  
"Urknall-Kosmologie-Elemententstehung - ein Überblick"
### 9. Outgoings: Foreign Research Visits of Institute Members

<table>
<thead>
<tr>
<th>Member</th>
<th>Dates</th>
<th>Institute and Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>I. Beinik</td>
<td>18.07.2010 - 27.07.2010</td>
<td>CINAM-CNRS, Marseille, (Frankreich)</td>
</tr>
<tr>
<td></td>
<td>15.09.2010 - 24.09.2010</td>
<td>Institute of Physics, National Academy of Science of the Czeck Republik</td>
</tr>
<tr>
<td></td>
<td>20.10.2010 - 27.10.2010</td>
<td>Institute of Semiconductor Physics, NAS Ukraine (Ukraine)</td>
</tr>
<tr>
<td>M. Erko</td>
<td>08.03.2010 - 15.03.2010</td>
<td>Elektronenspeicherring BESSY II am Helmholtz-Zentrum Berlin (HZB) (Deutschland), European Light Sources Activities - Synchrotrons and Free Electron Lasers (ELISA) (Italien)</td>
</tr>
<tr>
<td></td>
<td>22.03.2010 - 31.03.2010</td>
<td>Hahn-Meitner-Instituts Berlin (HMI) am Helmholtz-Zentrum Berlin (HIZB) (Deutschland), Initiative for Neutron Scattering and Muon Spectroscopy NMI3 (Belgien)</td>
</tr>
<tr>
<td></td>
<td>19.10.2010 - 26.10.2010</td>
<td>The European Synchrotron Radiation Facility (ESRF) (Frankreich)</td>
</tr>
<tr>
<td>M. Hartmann</td>
<td>16.04.2010 - 26.04.2010</td>
<td>Max-Planck-Institut für Kolloid- und Grenzflächenforschung (Deutschland)</td>
</tr>
<tr>
<td></td>
<td>02.06.2010 - 09.06.2010</td>
<td>Max-Planck-Institut für Kolloid- und Grenzflächenforschung (Deutschland)</td>
</tr>
<tr>
<td></td>
<td>09.07.2010 - 19.07.2010</td>
<td>Max-Planck-Institut für Kolloid- und Grenzflächenforschung (Deutschland)</td>
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<tr>
<td>M. Kratzer</td>
<td>03.10.2010 - 09.10.2010</td>
<td>Institute of Semiconductor Physics, NAS Ukraine (Ukraine)</td>
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<tr>
<td></td>
<td>27.03.2011 - 31.03.2011</td>
<td>O.O.Chuiko Institute of Surface Chemistry, Kiev (Ukraine)</td>
</tr>
<tr>
<td></td>
<td>03.07.2011 - 08.07.2011</td>
<td>Institute of Physics, National Academy of Science of the Czeck Republik</td>
</tr>
<tr>
<td></td>
<td>08.05.2011 - 16.05.2011</td>
<td>Berliner Elektronenspeicherring-Gesellschaft für Synchrostrahlungm.b.H., European Light Sources Activities (ELISA); supported by the EU - Research Infrastructure Action under the FP7 Programme (Italien)</td>
</tr>
<tr>
<td></td>
<td>14.06.2011 - 20.06.2011</td>
<td>Synchrotron ELETTRA, Sincrotrone Trieste (Italien)</td>
</tr>
<tr>
<td></td>
<td>11.03.2010 - 15.03.2010</td>
<td>Berliner Elektronenspeicherring-Gesellschaft für Synchrostrahlungm.b.H., DFG Schwerpunkt SPP 1420 (Deutschland)</td>
</tr>
<tr>
<td></td>
<td>19.06.2010 - 26.06.2010</td>
<td>European Synchrotron Radiation Facility - ESRF (Frankreich)</td>
</tr>
<tr>
<td>Name</td>
<td>Dates</td>
<td>Institution / Location</td>
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<tr>
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<tr>
<td>J. Oswald</td>
<td>01.08.2010 - 09.08.2010</td>
<td>Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung.m.b.H., European Light Sources Activities (ELISA) (Italien); supported by the EU - Research Infrastructure Action under the FP7 Programme</td>
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<td></td>
<td>20.06.2011 - 04.07.2011</td>
<td>Chiba University (Japan)</td>
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<td>30.10.2011 - 18.11.2011</td>
<td>Chiba University (Japan)</td>
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<td></td>
<td>17.01.2010 - 30.01.2010</td>
<td>Chiba University (Japan)</td>
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<tr>
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<td>14.11.2010 - 21.11.2010</td>
<td>Chiba University (Japan)</td>
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<tr>
<td>A. Pavitschitz</td>
<td>15.09.2010 - 24.09.2010</td>
<td>Institute of Physics, National Academy of Science of the Czeck Republik</td>
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<tr>
<td>Q. Shen</td>
<td>15.01.2011 - 19.01.2011</td>
<td>CINAM-CNRS, Marseille, (Frankreich)</td>
</tr>
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<td></td>
<td>03.07.2011 - 08.07.2011</td>
<td>Institute of Physics, National Academy of Science of the Czeck Republik</td>
</tr>
<tr>
<td>C. Teichert</td>
<td>15.04.2010 - 21.04.2010</td>
<td>Institute of Physics, National Academy of Sciences, Ukraine (Ukraine)</td>
</tr>
<tr>
<td></td>
<td>24.06.2010 - 02.07.2010</td>
<td>CINAM-CNRS, Marseille, (Frankreich)</td>
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<tr>
<td></td>
<td>11.10.2011 - 14.10.2011</td>
<td>Institute of Physics, National Academy of Science of the Czeck Republik</td>
</tr>
<tr>
<td></td>
<td>13.02.2011 - 19.02.2011</td>
<td>CINAM-CNRS, Marseille, (Frankreich)</td>
</tr>
</tbody>
</table>
10. Conference Organisation

Friedemar Kuchar, G. Bauer, W. Jantsch

Christian Teichert

Oskar Paris
- Synchrotron Resarch in Austria with particular consideration of the European Synchrotron Radiation Facility ESRF, 2. Austrian Synchrotron Radiation User Meeting 18.10.2011, Wien, Austria
- International Workshop and School: NESY European Winterschool on Neutrons and Synchrotron Radiation, 6.-12.3.2011, Planneralm, Austria

11. University Administration

Ronald Meisels
- Curriculum Kommission „Doktoratsstudium“

Josef Oswald
- Institute of Physics: Vice Chair
- Senat (Vice Chair)
- Betriebsrat (Vize Chair/Chair)
- Universitätsgewerkschaft wissenschaftliches Personal, Bundesvertretung 13 der GÖD (Vice Chair)
- Verhandlungsteam der GÖD für den Universitätskollektivvertrag (Member)
- Berufungskommission Mechanik (Member)
- Mitglied des Satzungsarbeitskreises des Rektors
- Mitglied der Wahlkommission für die Senatswahl

Oskar Paris
- Institute of Physics: Chair
- Vizestudiendekan (Vice Dean): since October 2011
- Senat (Member)
- Strategieprozess der Montanuniversität (Member of the Core Team): July-Dec. 2011
- Berufungskommission Werkstoffkunde und Prüfung der Kunststoffe (member): 2010
- Berufungskommission Funktionale Werkstoffe und Werkstoffsysteme (member): 2010
- Habilitationskommission Puschnig (Member):2010
- Habilitationskommission Grün (Member): 2011
- Habilitationskommission Motz (Chair): 2011/2012

Christian Teichert
- Curriculum Kommission „Werkstoffwissenschaften“ (Member)
- Strategieprozess der Montanuniversität (Member): July-Dec. 2011
- Berufungskommission Werkstoffkunde und Prüfung der Kunststoffe (Member): 2010
- Habilitationskommission Puschnig (Member):2010
- Habilitationskommission Motz (Member): 2011/2012
12. Advisory- & Editorial Boards, Review Committees, Membership, etc.

Ronald Meisels
- Member IEEE (Institute of Electrical and Electronic Engineers)

Josef Oswald
- Gutachtertätigkeit BMWF/ÖAD

Oskar Paris
- HASYLAB (DESY, Hamburg): Project Review Panel (until 2010)
- Helmholtz Center Berlin (HZB): Scientific Selection Panel
- FRM II Munich: Proposal Committee Member
- COST Action MP0601: Management Committee Member
- BMWF Gutachterausschuss 2010-2013: Erforschung kondensierter Materie an Großforschungsanlagen.
- Review Committee Member of the “Helmholtz high data-rate processing and analysis initiative” (March 2010)
- Review Committee Member of the “ESRF Update Program, Beamline UPBL9a” (May 2011)
- Gutachtertätigkeit für Professuren (Boku Wien, Univ. Hamburg), Doktorarbeiten (TU Graz, Uni Wien, TU Berlin, Humboldt Univ. Berlin, Univ. des Saarlandes), und für viele international Zeitschriften
- Chair of the “ESRF Beirat” of the Austrian Academy of Science (since Oct. 2010)
- Austrian ESRF Council Observer (since Oct. 2011)

Christian Teichert
- Mitglied Organisationskomitee Rathen (Deutschland)
- Vorsitzender Organisationskomitee, Leuchturm „Nanogrowth“ im NANO_NET Styria,
- Gutachtertätigkeit ÖAD, Czech, Swiss and Canadian Science Foundations, Gutachtertätigkeit für Professuren (Univ. Enschede, NL), Promotionskommission (TU Graz, Univ. Nova Gorica, Slo.)
- Mitglied Int. Steering Committee Int. Vacuum Conf. 18 & ICN+T 2010, Beijing
- National representative and since 2010 Secretary of the Nano Science Devision, IUVSTA
Picture Galery

Farewell- and inaugural lectures from F. Kuchar and O. Paris

Friedemar Kuchar, Rector Wolfhard Wegscheider, Oskar Paris

16th International Winterschool on New Developments in Solid State Physics: Low Dimensional Systems "Mauterndorf 2010"

F. Kuchar with the Mayor of Mauterndorf

Klaus von Klitzing (Nobelpreisträger 1985)

Postersession
Igor Beinik receives the Anton Paar Science Award in Physics 2011 in Lausanne, Switzerland

Ski excursion
Participants of the “International Workshop and School: NESY European Winterschool on Neutrons and Synchrotron Radiation”, Planneralm, 6 – 12 March 2011, organized by the Institute of Physics.
Small angle scattering image from nanoporous silica monoliths obtained by nanocasting of spruce latewood