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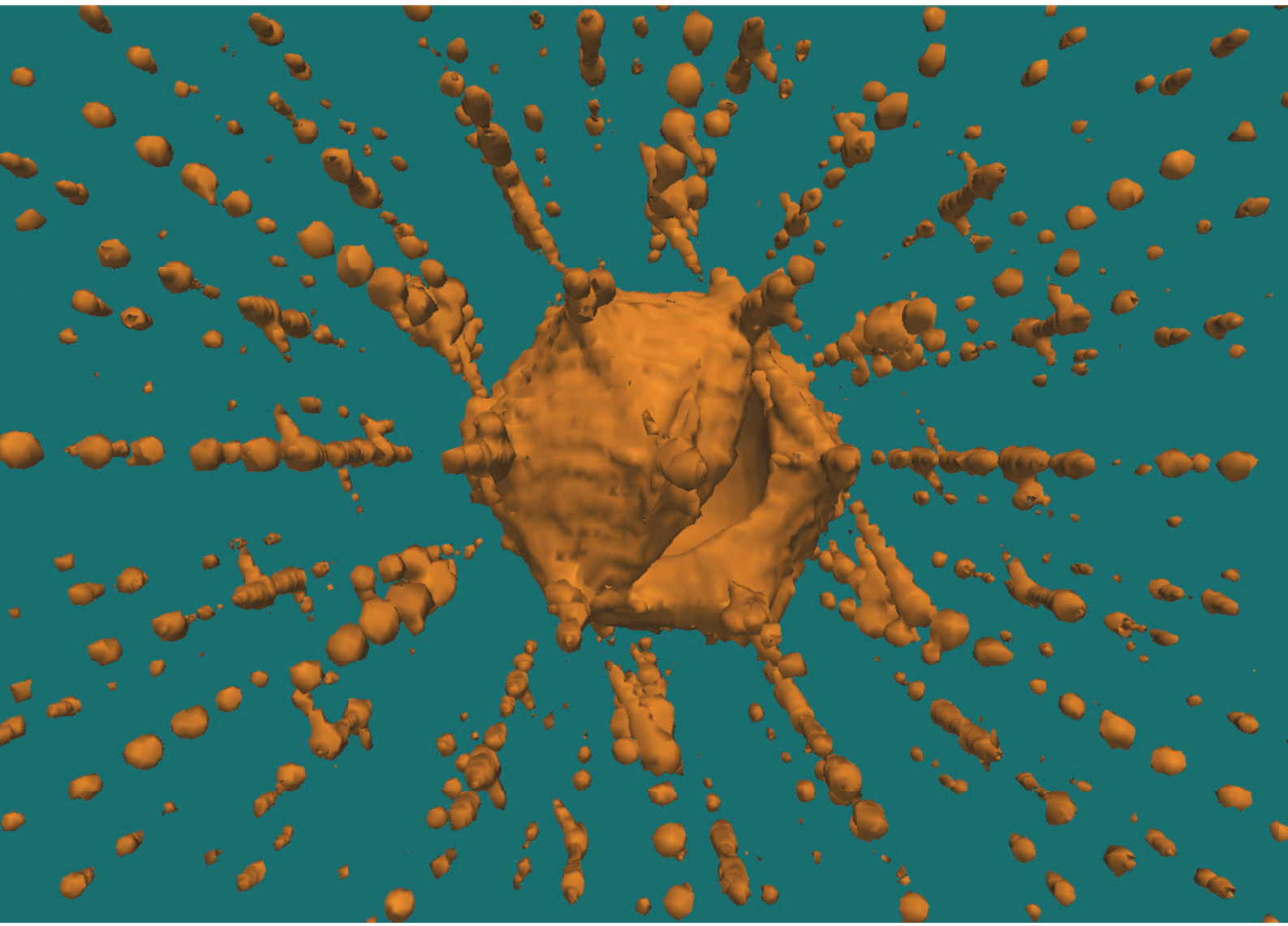

BI - ANNUAL REPORT
2012 and 2013

Institutsausflug Lurgrotte (Institute excursion to Lurgrotte)

Impressum

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Cover picture:
3D reciprocal space map of a colloidal crystal consisting of self assembled Bi nanoparticles

Institut für Physik

Montanuniversität Leoben

BI-ANNUAL REPORT

2012/2013

CONTENTS Page

Preface

Dear partners and friends,

it is a pleasure to present you this overview of the research- and teaching activities of the Institute of Physics within the years 2012 and 2013. As already two years ago we decided to stick on a bi-annual reporting scheme which seems more adequately reflecting the scientific progress and organizational changes of a university institute without unnecessary replications.

At the heart of the bi-annual report are the research reports summarizing the scientific achievements of the four independent research groups. Our scientific mission is to conduct high-level basic research in the field of "Physics of Functional Materials for Electronics, Optics and Energy". While electronics and optics have a long tradition at the institute, the energy thematics is - exept of some long-term activities on solar cell materials - rather recent. A strong focus on nanoporous materials has meanwhile been established, such systems being relevant for the storage of chemical or electrical energy, for instance. Another hot research topic evolving quite successfully at the institute is around the promising 2D-material graphene. Further research activities include work on biological, bioinspired and bio-based materials, on functional nanoparticles and nanocrystals, as well as on light- and electron transport under the influence of magnetic fields. More applied projects deal with whole devices such as varistors or supercapacitors, or with the use of physical methods to fragment rocks (by microwave radiation) or to separate mineral particles (tribolelectrically). The publication output resulting from these activities in the reporting period is excellent, amounting to more than 60 publications. Almost 50 of them are original papers in SCI listed journals, amongst them some "high-impact" publications in, e.g., *Nature Scientific Reports, Journal of the American Chemical Society* or *Advanced Functional Materials*. It is worth mentioning that with this publication record we contribute almost 15% of the total annual SCI publication output at the Montanuniversität. In addition to the written output, far more than 100 presentations were delivered at scientific conferences, and several awards were granted to young scientist from the institute.

Modern research requires money, the acquisition of research funds becoming increasingly competitive in particular in the basic science disciplines. In this light I am very proud that several multi-annual research projects with at least one project-financed scientific coworker and a total budget of more than one Million Euro could be executed at the institute, with two new projects starting within the reporting period. In addition - besides several smaller (e.g. ÖAD) projects – almost two full months of measurement time at large scale facilities for e.g. synchrotron- and neutron radiation were granted to institute members within an internationally competitive peer review process. Just to explain the significance of this success: a company conducting proprietary research would have to pay around 10.000 Euro for each beamtime day, and hence, this would amount to an equivalence of more than half a Million Euro of funding.

The personnel situation of the institute is more or less stable at around 20 staff, with roughly half of the scientific coworkers being financed from projects. After more than one year with only three faculty assistants, we are very happy to be back to four assistants since October 2013. This was absolutely necessary in view of the continuously increasing number of freshmen students at our university, which continues to shift the duties of the faculty staff towards teaching at the expense of research. The high teaching load is demonstrated for instance by the increase of the number of teaching classes by more than 20% and the total number of exams by almost 50% since the last reporting period. It will certainly become increasingly difficult to keep the right balance between teaching and research in the future. Nonetheless, I see it as my major responsibility to facilitate both, high-quality education and cutting-edge research at the Institute of Physics. I really hope that the future science political developments in Austria will enable us to further stick to this Humboldt's "Unity of Research and Teaching" principle.

The progress and achievements compiled in this bi-annual report 20012-2013 would not have been possible without highly motivated coworkers and many cooperation partners from all over the world. I am very grateful to all members of the institute for their engagement and to you as partners and promoters for the continuous support. I hope you enjoy reading through this report and keep in touch with the Institute of Physics.

Univ.-Prof. Dr. Oskar Paris

September 2014

Personnel

Faculty: Science and Teaching

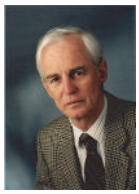
Professors

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

Ao.Univ.-Prof. Dr. Josef OSWALD
(Vice-Chair until 7/2013)

Ao.Univ.-Prof. Dr. Christian TEICHERT
(Vice-Chair since 7/2013)

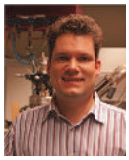
Ao.Univ.-Prof. Dr. Ronald MEISELS



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

Assistants

Dr. Markus HARTMANN
Assistant/Senior Researcher



Dr. Rainer LECHNER
Assistant/Senior Researcher

Dr. Markus KRATZER
Assistant/Senior Researcher

Dipl. Phys. Maxim ERKO
Assistant/PhD Student
(until June 2012)

Dipl. Ing. Roland MORAK
Assistant/PhD Student
(since October 2013)

Faculty: Administration and Technical Support

Heide KIRCHBERGER
(Secretary)

Peter MOHARITSCH
(Mechanical Engineer)

Magdalena OTTRIN
(Secretary)

Ing. Heinz PIRKER
(Electrical Engineer)

Research Associates and Students workers

Dr. Roland BRUNNER
Postdoc (until 5/2012)

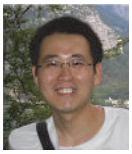
Dr. Gerhard POPOVSKI
Postdoc

Dr. Parvin SHARIFI
Postdoc (since 10/2012)

Dipl.Ing. Christian GANSER
Doctoral student

Dipl.Ing. Andreas PAVITSCHITZ
Doctoral student

Dipl.Ing. Stefan LORBEK
Doctoral student



Dipl.Ing. Quan SHEN
Doctoral student

MSc. Seyedsoran NABAVI
Doctoral student

Mgr inz. Monika Mirkowska
Doctoral student, joint with Chair of Mineral Processing (since 8/2012)

Patrice KREIML
Student Worker,
Diploma thesis (since 12/2013)

Lin Wang
Student Worker,
Diploma thesis (until 3/2012)

Mario LUGGER
Student Worker,
Diploma thesis (until 2/2012)

Christian PREHAL
Student Worker,
Diploma thesis (since 04/2013)

Max BURIAN
Diploma thesis (since 08/2013)

Reinhold J. WARTBICHLER
Student Worker (03-09/2013)

Catherina CZIBULA
Student worker (since 09/2013)

2. Teaching

2.1 Courses held in the academic years 2011/20012 and 2012/2013

Winter Term 2011/2012

Number	Title	Hours per week / Type		Lecturer
460.129	Anleitung zu wissenschaftlicher Arbeit auf dem Gebiet der Physik von Halbleitern und Nanosystemen	10	PV	Kuchar F, Meisels R, Oswald J, Paris O, Teichert C
460.112	Ausgewählte Problemstellungen der Quantenphysik	2	VO	Oswald J
460.060	Bauprinzipien biologischer Materialien	1,5	VO	Paris O
460.111	Einführung in die Oberflächen- und Dünnschichtprozesse	2	VO	Teichert C
460.094	Halbleiterwerkstoffe	2	VO	Meisels R, Teichert C
460.104	Herstellung einkristalliner Schichten - Epitaxie	2	VO	Kratzer M, Teichert C
460.066	Industrielle Herstellungstechniken der Mikroelektronik	2	VO	Noll H
460.003	Konversatorium zu Physik I	1	KV	Paris O
460.067	Mechanisch-Physikalische Messtechnik	1	VO	Oswald J
460.072	Physik der Mikro- und Nanoelektronik-Bauelemente	2	VO	Meisels R
460.005	Physik IA	2	VO	Paris O
460.006	Physik IB	2	VO	Paris O
460.030	Physik Praktikum I *(15 groups)*	2	UE	Ganser C, Hartmann M, Hyden W, Kratzer M, Lechner R, Meisels R, Oswald J, Popovski G, Teichert C
460.001	Rechenübungen zu Physik IA und IB *(16 groups)*	2	UE	Brunner R, Erko M, Glushko O, Hartmann M, Hofstätter M, Kratzer M, Lechner R, Meisels R, Milko M, Nevosad A, Puschnig P, Steiner-Luckabauer C, Teichert C
460.004	Repetitorium Physik I	1	RP	Paris O
460.022	Repetitorium Physik I	1	RP	Oswald J
460.121	Seminar aus Halbleiterphysik und Nanotechnologie	2	SE	Meisels R, Oswald J, Paris O, Teichert C
460.076	Übungen zu Charakterisierung von Werkstoffen der Elektronik	2	UE	Lechner R, Meisels R, Oswald J, Paris O, Teichert C

Summer Term 2012

Number	Title	Hours per week / Type		Lecturer
460.132	Anleitung zu wissenschaftlicher Arbeit auf dem Gebiet der Physik von Halbleitern und Nanosystemen	10	PV	Kuchar F, Meisels R, Oswald J, Paris O, Teichert C
460.108	Anwendung von Computersimulationen in der Metall- und Biophysik	2	VO	Hartmann M
460.101	Elektronische und mechanische Eigenschaften von Heterostruktur-Bauelementen	2	VO	Kasper E
460.460	Exkursion: Synchrotronstrahlung in der Materialforschung	2	EX	Paris O
460.110	Grundprinzipien der Quantenphysik	2	VO	Oswald J
460.105	Magnetische Eigenschaften von Nanowerkstoffen	2	VO	Lechner R
460.010	Physik II	2	VO	Paris O

460.016	Physik III	2	VO	Teichert C
460.054	*Physik Praktikum II (6 groups)*	2	UE	Erko M, Kratzer M, Lechner R, Meisels R, Oswald J
460.113	Physik von Fullerenen, Graphen und Carbon Nanotubes	2	VO	Teichert C
460.103	Rastersondentechniken zur Charakterisierung von Festkörperoberflächen	2	VO	Teichert C
460.009	Rechenübungen zu Physik II *(15 groups)*	1	UE	Glushko O, Hartmann M, Kirchlechner C, Kratzer M, Lechner R, Lorbek S, Meisels R, Nevosad A, Oswald J, Popovski G
460.048	Rechenübungen zu Physik III *(2 groups)*	1	UE	Kratzer M, Teichert C
460.004	Repetitorium Physik	1	RP	Paris O
460.022	Repetitorium Physik I	1	RP	Oswald J
460.122	Seminar aus Halbleiterphysik und Nanotechnologie	2	SE	Meisels R, Oswald J, Paris O, Teichert C
460.068	Übungen zu Mechanisch-Physikalische Messtechnik *(3 groups)*	2	UE	Ganser C, Meisels R, Oswald J
430.001	Werkstoffmodellierung auf atomarer Ebene	0,67	VO	Hartmann M
431.009	Übungen zu Werkstoffmodellierung auf atomarer Ebene	1	UE	Hartmann M
420.102	Einführung in die Werkstoffwissenschaft	0,25	SE	Paris O, Teichert C

Winter Term 2012/2013

Number	Title	Hours per week / Type		Lecturer
460.129	Anleitung zu wissenschaftlicher Arbeit auf dem Gebiet der Physik von Halbleitern und Nanosystemen	10	PV	Meisels R, Oswald J, Paris O, Teichert C
460.060	Bauprinzipien biologischer Materialien	1,5	VO	Paris O
460.111	Einführung in die Oberflächen- und Dünnschichtprozesse	2	VO	Teichert C
460.094	Halbleiterwerkstoffe	2	VO	Meisels R, Teichert C
460.104	Herstellung einkristalliner Schichten - Epitaxie	2	VO	Kratzer M, Teichert C
460.066	Industrielle Herstellungstechniken der Mikroelektronik	2	VO	Noll H
460.003	Konversatorium zu Physik I	1	KV	Paris O
460.067	Mechanisch-Physikalische Messtechnik	1	VO	Oswald J
460.072	Physik der Mikro- und Nanoelektronik-Bauelemente	2	VO	Meisels R
460.005	Physik IA	2	VO	Paris O
460.006	Physik IB	2	VO	Paris O
460.030	Physik Praktikum I *(12 groups)*	2	UE	CHartmann M, Lechner R, Meisels R, Oswald J, Teichert C
460.114	Quantenmechanik *(2 Gruppen)*	2,5	IV	Oswald J
460.001	Rechenübungen zu Physik IA und IB *(19 groups)*	2	UE	Angerer P, Bodor C, Ganser C, Glushko O, Hartmann M, Hofstätter M, Klünsner T, Kratzer M, Lechner R, Meisels R, Nabavi S, Popovski G, Renk O, Teichert C, Wurster S
460.004	Repetitorium Physik	1	RP	Paris O
460.022	Repetitorium Physik I	1	RP	Oswald J
460.121	Seminar aus Halbleiterphysik und Nanotechnologie	2	SE	Meisels R, Oswald J, Paris O, Teichert C
460.076	Übungen zu Charakterisierung von Werkstoffen der Elektronik	2	UE	Lechner R, Meisels R, Oswald J, Teichert C

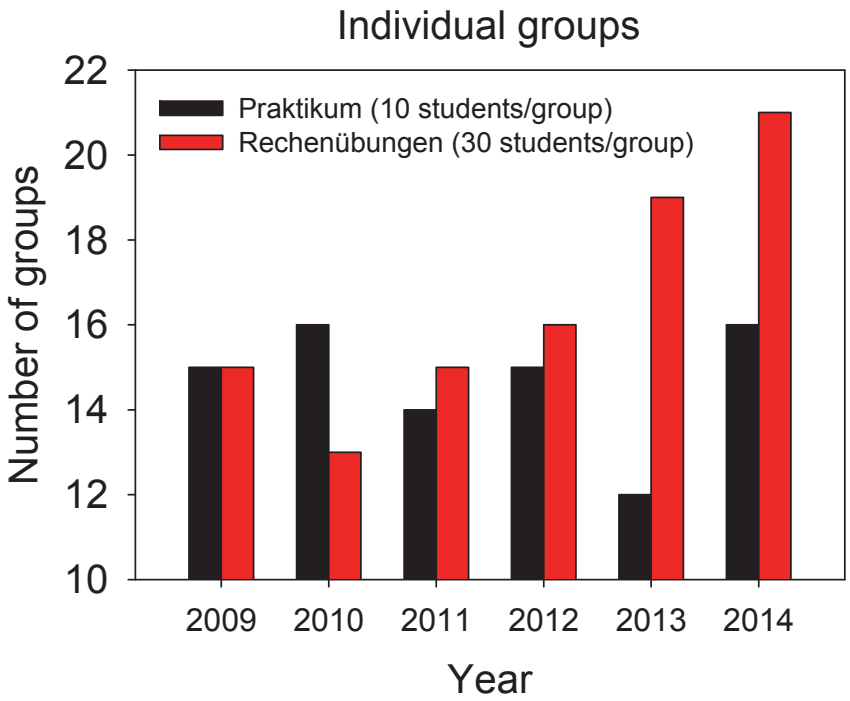
Summer Term 2013

Number	Title	Hours per week / Type		Lecturer
460.132	Anleitung zu wissenschaftlicher Arbeit auf dem Gebiet der Physik von Halbleitern und Nanosystemen	10	PV	Kuchar F, Meisels R, Oswald J, Paris O, Teichert C
460.108	Anwendung von Computersimulationen in der Metall- und Biophysik	2	VO	Hartmann M
460.102	Elektronische und mechanische Eigenschaften von Heterostruktur-Bauelementen	2	VO	Kasper E
460.110	Grundprinzipien der Quantenphysik	2	VO	Oswald J
460.105	Magnetische Eigenschaften von Nanowerkstoffen	2	VO	Lechner R
460.010	Physik II	2	VO	Paris O
460.016	Physik III	2	VO	Teichert C
460.054	*Physik Praktikum II (5 groups)*	2	UE	Hartmann M, Kratzer M, Lechner R, Meisels R
460.113	Physik von Fullerenen, Graphen und Carbon Nanotubes	2	VO	Teichert C
460.103	Rastersondentechniken zur Charakterisierung von Festkörperoberflächen	2	VO	Teichert C
460.009	Rechenübungen zu Physik II *(17 groups)*	1	UE	Angerer P, Bodor C, Gloggnitzer S, Glushko O, Hartmann M, Klünsner T, Kratzer M, Lechner R, Meisels R, Puchleitner R, Renk O
460.048	Rechenübungen zu Physik III *(1 group)*	1	UE	Teichert C
460.004	Repetitorium Physik	1	RP	Paris O
460.022	Repetitorium Physik I	1	RP	Oswald J
460.122	Seminar aus Halbleiterphysik und Nanotechnologie	2	SE	Meisels R, Oswald J, Paris O, Teichert C
460.100	Strukturforschung mit Röntgen- und Neutronenstreuung an Europäischen Großforschungsanlagen	2	UE	Keckes J, Paris O
460.460	Synchrotronstrahlung in der Materialforschung	2	EX	Lechner R, Paris O
460.068	Übungen zu Mechanisch-Physikalische Messtechnik *(4 groups)*	2	UE	Ganser C, Meisels R, Oswald J
430.001	Werkstoffmodellierung auf atomarer Ebene	0,67	VO	Hartmann M
431.101	Übungen zu Werkstoffmodellierung auf atomarer Ebene	1	UE	Hartmann M
420.102	Einführung in die Werkstoffwissenschaft	0,25	SE	Paris O, Teichert C

2.2 Lectors: External help with teaching

Teaching is mainly covered by the faculty staff members. However, to cover the exercises and the practical training in Physics for the ever increasing number of freshmen students we have to rely more and more on the help from motivated lecturers. This is meanwhile becoming a serious problem since the increasing number of students (see graphics below), financial limitations of the University, and controversies with funding agencies makes it increasingly difficult to find proper teaching personnel. We are gratefully for the help from research associates from our Institute, from other Chairs of the MUL, and from external lecturers, e.g., from the Erich Schmid Institute of the Austrian Academy of Sciences (ESI) or from the Materials Center Leoben (MCL).

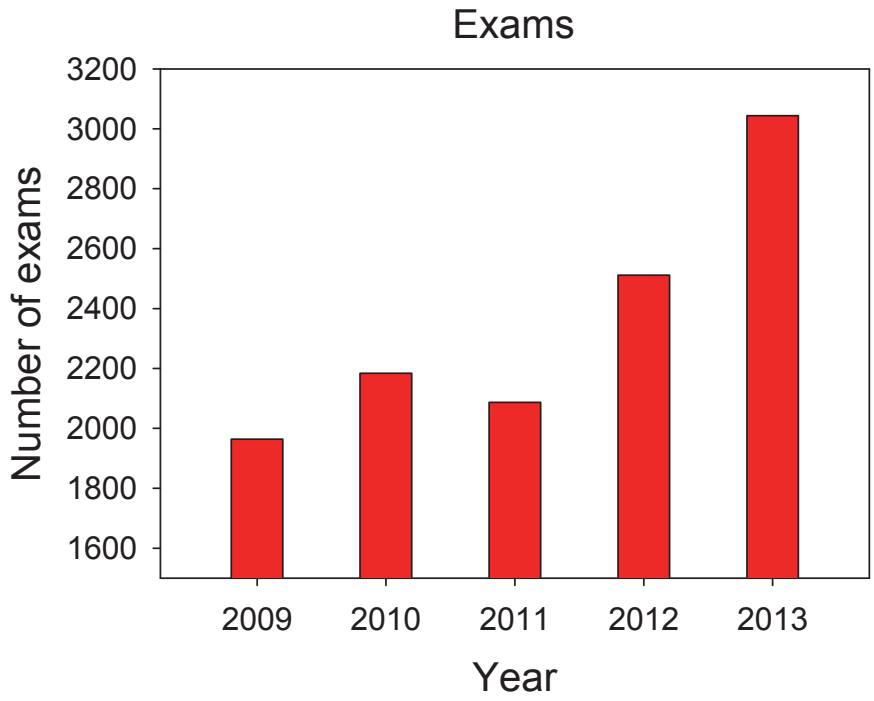
- Dr. R. Brunner, Dr. O. Glushko, Dipl. Phys. S. Lorbek, MSc. S. Nabavi, Dipl. Ing. A. Pavitschitz, Dr. G. Popovski, Institut für Physik
- Dr. M. Hofstätter, Institut für Struktur- und Funktionskeramik
- Dr. C. Steiner-Luckabauer Lehrstuhl für Angewandte Geophysik
- Dr. M. Milko, Dr. P. Puschnig, Lehrstuhl für Atomistic Modelling
- Dr. P. Angerer, Dr. Brunner, Dr. T. Klünsner, Materials Center Leoben
- Dr. Kirchlechner, Dipl. Ing. S. Wurster, Lehrstuhl für Materialphysik
- Dipl. Ing. W. Hyden, Lehrstuhl für Geophysik
- Dipl.Ing. C. Bodor, Lehrstuhl für Spritzgießen von Kunststoffen
- Dipl.Ing. S. Gloggnitzer, Lehrstuhl für Werkstoffkunde und Prüfung der Kunststoffe
- Univ.Prof. Dr. E. Kasper, Institut für Halbleitertechnik, Universität Stuttgart, Germany
- Dr. H. Noll, Fachhochschule Wr. Neustadt



Development of the number of teaching classes (groups) in the winter term for exercises and practical training in Physics. While the number of practical training groups remains roughly constant, the number of classes for the exercises, and thus the number of required external lectors, clearly increases.

2.3 Exams

LV.Nr.	Titel	2012	2013
460.001	Rechenübungen zu Physik I	485	627
460.002	Physik I	83	1
460.003	Konversatorium zu Physik I	56	0
460.004	Repetitorium Physik I	23	14
460.005	Physik IA	463	703
460.006	Physik IB	239	394
460.009	Rechenübungen zu Physik II	402	494
460.010	Physik II	238	331
460.016	Physik III	63	39
460.030	Übungen zu Physik (I)	150	123
460.048	Rechenübungen zu Physik III	52	31
460.054	Übungen zu Physik (II)	61	48
460.060	Bauprinzipien biologischer Materialien	32	36
460.066	Industrielle Herstellungstechniken der Mikroelektronik	3	0
460.067	Mechanisch-Physikalische Messtechnik	38	49
460.068	Übungen zu Mechanisch-Physikalische Messtechnik	33	38
460.072	Physik der Mikro- und Nanoelektronik-Bauelemente	1	1
460.076	Übungen zu Charakterisierung von Werkstoffen der Elektronik	0	1
460.077	Physikalische und Technische Grundlagen von Sensoren	1	0
460.094	Halbleiterwerkstoffe	34	26
460.100	Strukturforschung mit Röntgen- und Neutronenstreuung an Europäischen Großforschungsanlagen	0	6
460.101	Elektronische und mechanische Eigenschaften von Heterostruktur-Bauelementen	0	0
460.103	Rastersondentechniken zur Charakterisierung von Festkörperoberflächen	12	6
460.104	Herstellung einkristalliner Schichten - Epitaxie	0	2
460.105	Magnetische Eigenschaften von Nanowerkstoffen	1	0
460.108	Anwendung von Computersimulationen in der Metall- und Biophysik	3	0
460.110	Grundprinzipien der Quantenphysik	1	0
460.111	Einführung in die Oberflächen- und Dünnschichtprozesse	7	3
460.113	Physik von Fullerenen, Graphen und Carbon Nanotubes	2	6
460.114	Quantenmechanik	0	49
460.121	Seminar aus Halbleiterphysik und Nanotechnologie	1	1
460.122	Seminar aus Halbleiterphysik und Nanotechnologie	0	0
460.129	Anleitung zu wissenschaftlicher Arbeit auf dem Gebiet der Physik von Halbleitern und Nanosystemen	1	0
430.101	Übungen zu Werkstoffmodellierung auf atomarer Ebene		
430.001	Werkstoffmodellierung auf atomarer Ebene	2	3
460.460	Exkursion: Synchrotronstrahlung in der Materialforschung	21	10
	Diplomprüfungen	2	1
	Rigorosen	1	1
	Total number of exams	**2.511**	**3.044**

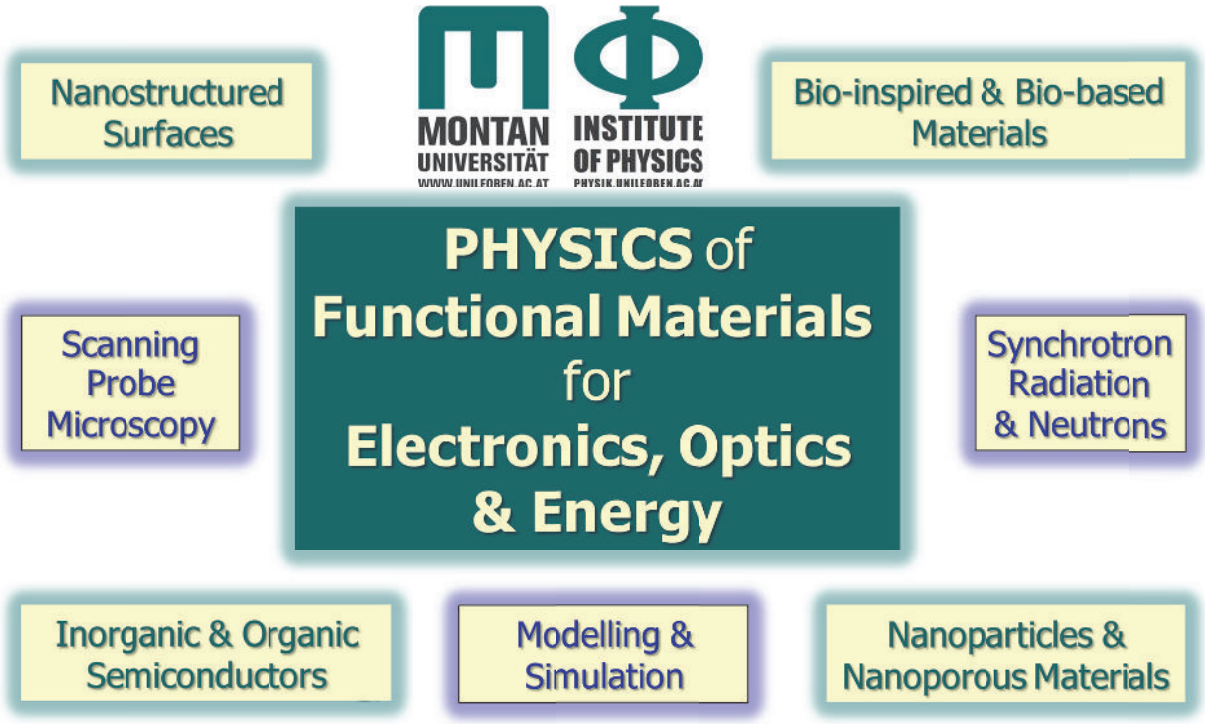


Development of the annual number of exams taken by the institute of physics. Asuming 15 minutes as an absolute minimum time for each single exam, 3000 exams amount to 750 hours of examination, which comes to 94 full working days.

3. Research

3.3 Research reports

Research at the Institute of Physics is mainly dedicated to basic science in materials physics, with emphasis on nanostructured surfaces, semiconductor physics including optics and electronic transport, nanoparticles and nanoporous materials, as well as biological, bio-inspired and bio-based systems. (Nano-) structure and functional properties of a wide range of materials such as graphene, semiconductor nanoparticles, ordered nanoporous silica, or paper fibers are in the focus of current research. Two major experimental methods are employed namely scanning probe microscopy and scattering techniques, including the use of synchrotron- and neutron radiation at large-scale facilities. Experimental work is complemented by a range of numerical simulation tools such as atomistic Monte Carlo simulations, finite difference time domain (FDTD) calculations, or quantum mechanical simulations.



Our research is structured in four independent research groups each lead by one of the four Professors of the Institute.

Nanomaterials and Scattering: Oskar Paris
Max Burian, Maxim Erko, Markus A. Hartmann, Rainer T. Lechner, Soran Nabavi, Roland Morak, Gerhard Popovski, Christian Prehal, Parvin Sharifi

Surface Physics and Scanning Probe Microscopy: Christian Teichert
Catherina Czibulka, Christian Ganser, Jakob Genser, Stefan Klima, Markus Kratzer, Patrice Kreiml, Michael Lasnik, Monika Mirkowska, Quan Shen, Reinhold J. Wartbichler.

Photonics and Nanoelectronics: Ronald Meisels
Roland Brunner, Friedemar Kuchar

Simulation Electric Transport: Josef Oswald

The following pages compile the research reports from these groups in the reporting period 2012/2013. Furthermore, in an Epilogue, our Professor Emeritus Friedemar Kuchar gives an outlook on future trends in micro- and nanoelectronics.

Computational Materials Science

Markus A. Hartmann, Soran Nabavi
markus.hartmann@unileoben.ac.at

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 bonding is an effective strategy to increase the toughness of natural materials that is used in a large variety of biological materials like bone and wood as well as in some softer biological fibers e.g. silk, mussel byssus threads and the whelk egg capsule. Sacrificial bonds (SBs) are weaker than the covalent bonds that hold the structure together. Thus, upon loading the SBs break before the backbone ruptures revealing hidden length which is the microscopic mechanism providing the material with its exceptional toughness. Furthermore, in contrast to covalent bonds SBs are reversible and may reform upon release of the load. The reversibility ensures that after some time the material regains its original mechanical properties offering a mechanism of self-healing.
Different types of bonds like, metal-coordination bonds, hydrogen bonds, etc. are known to act as SBs. Metal-coordination bonds are found in byssal threads providing them with a high extensibility of over 100%, high stiffness and toughness. Furthermore, they allow adhering to different substrates even in a wet environment. It is these impressive properties that drive the demand to transfer some of these natural design principles into technological applications, like the development of strong biocompatible surgical adhesives, of implantable drug-eluting devices in human blood vessels capable of withstanding blood flow or to design super tough hydrogels. Nevertheless, the transfer of these natural design principles into application first demands the detailed understanding of the biological system. Due to the inherent complex structure of biological systems, computer simulations are a promising tool to make the complicated system theoretically tractable and to help to interpret experimental findings.
The investigated model consists of a covalently bonded linear chain with some of the monomers labeled "sticky". Two sticky sites can form a sacrificial bond that can thermally induced open and close reversibly.
Figure 1 shows the load-displacement curve for a single chain with 4 sticky sites. In this system three different topologies of SBs may form: the independent, nested and pseudoknotted type. It has been shown that the topology determines the position of the force peaks, while the efficacy of the sacrificial bonds (the height of the peaks) is reduced due to thermal fluctuations of the backbone [1]. As indicated in the figure the nested configuration is responsible for peak (I), the pseudoknotted topology for peak (IIA) and the independent topology determines peak (IIB). All of the topologies contribute to the peak (III), while peak (IV) is the trivial contribution due to backbone stretching.

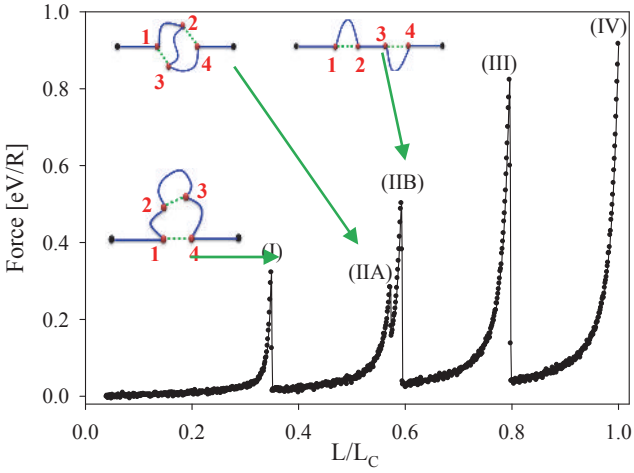


Fig. 1 *Load-displacement curve for* $N = 50$ *and* $k_B T = 25\ meV$.

Furthermore, simulations mimicking cyclic loading experiments revealed an asymmetry between loading and unloading resulting in a pronounced hysteresis. This hysteresis area is a measure of the dissipated energy per loading cycle and strongly depends on the number of SBs in the chain as well as on their topology. Furthermore, since the mechanical properties strongly depend on the topology of the SBs, the speed of unloading determines the mechanical properties of the second loading cycle. A slow return favors the independent topology, while a fast return also allows for the mechanically superior nested and pseudoknotted structures.
Another investigation concerns the influence of the spatial arrangement of the SBs on the mechanical properties of the chain. Figure 2 shows load-displacement curves for a single chain with 12 sticky

sites that are differently arranged along the backone. One configuration is completely random. In the patches configuration the sticky sites are concentrated at the two ends of the polymer, while the middle region is sticky site free. Although the total number of SBs is the same for both configurations the mechanical properties like the strength (maximum force) and apparent stiffness are considerably different [2].

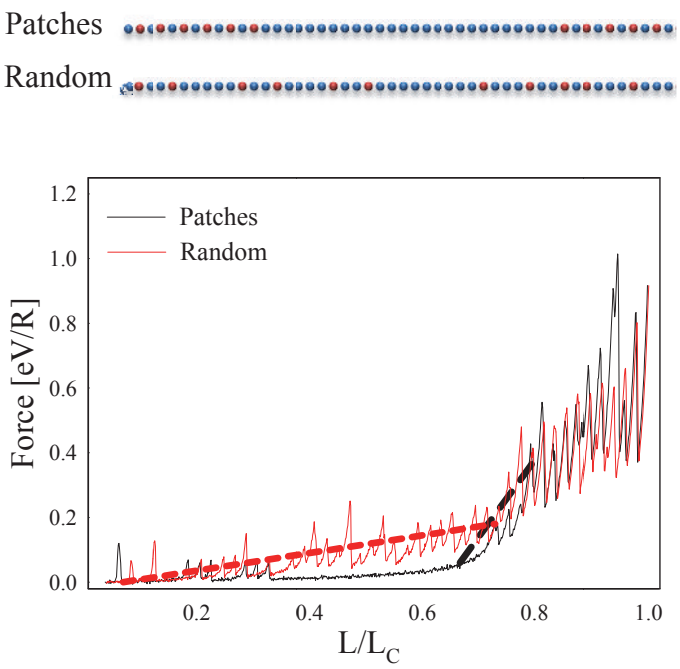


Fig. 2 *Load-displacement curves for two different distributions of sticky sites (patches and random) and* $N = 50$ *and* $k_B T = 25\, meV$*. The dashed lines indicate the apparent stiffness of the materials defined as the mean slope of the first part of the load-displacement curve. In the top part of the figure a sketch of the different arrangements of sticky sites is shown (sticky sites are shown in red, non-sticky sites in blue).*

Future investigations will include the effect of sacrificial bonding in multi chain systems (see fig. 3). Additional to intra-chain bonds SBs may now also form inter-chain bonds between different chains, which dramatically changes the mechanical properties of such systems.

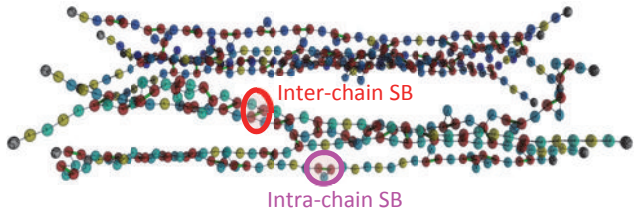


Fig. 3 *A snapshot of the multi chain system with 9 chains each consisting of 50 beads with 24 sticky sites each. Open sticky sites are shown in yellow, closed SBs are shown in red, first and last bead of each chain is depicted in gray and non-sticky sites in blue.*

In particular the influence of SB density and grafting density on the mechanical behavior of such multi chain systems will be investigated. While intra-chain SBs determine the toughness of the system, the presence of inter-chain SBs is responsible for an elevated stiffness.

Funding:
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Cooperation:
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2) Mechanical properties of carbon nanostructures
Carbon nanostructures, like the planar graphene and its curved offspring nanotubes and fullerenes are among the stiffest and strongest materials ever discovered. Additionally they are of extremely low weight. It is these fascinating properties that make these structures promising candidates to revolutionize structural mechanics. Nevertheless, to fully exploit the benefits of carbon nanostructures in technological applications it is inevitable to fully understand the mechanical behavior of graphene that is strongly influenced by its intrinsic 2-dimensional structure. One of the key questions in this context concerns the determination of the thickness of graphene. This is especially important for the investigation of larger structures composed of many layers of graphene using large scale continuum methods that describe graphene as a thin, elastic shell. Such a classical shell is characterized by three independent parameters: the elastic modulus and the Poisson ratio of the material and the thickness of the shell. The question that naturally arises is what thickness can be attributed to a 2-dimensional structure? The values proposed in literature span an extremely wide range of more than one order of magnitude. This situation was termed "Yakobson paradox". In [3] computational mechanical tension and compression tests as well as bending tests were done on graphene to determine its relevant mechanical parameters. It was shown that the elastic modulus and the Poisson ration can be accurately determined and that the results are in agreement with measurements presented in literature [4]. Most important it was shown that the effective thickness of graphene attains a constant value of approximately 1.32 Å when graphene is larger than 50 Å and that this thickness effectively decreases when graphene is shorter (see fig. 4a). This effect can be attributed to the breakdown of continuum mechanics for structures composed of too few atoms.
Another question related to the properties of graphene concerns the mechanical properties and stability of shell-like structures like carbon onions that are composed of many concentric layers of monolayer graphene. To adequately describe the effect of these non-covalently bonded layers van-der Waals interactions have to be included in the theoretical

modeling. Due to the different number of atoms in adjacent layers the correct formulation of the van der Waals interactions in continuum mechanics is challenging [5]. It is the pressure due to van der Waals interactions that is responsible for the emergence of a structural instability that limits the size of carbon onions [6].

Upon application of hydrostatic pressure carbon nanotubes initially homogeneously shrink in radius. When the pressure exceeds the critical pressure the structure ovalizes showing a hard-to-soft transition (see fig. 4b). This transition can be experimentally monitored by measuring the shift in Raman frequencies upon application of the pressure. Additional computational investigations help to interpret these experimental findings [7].

Cooperation:

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David J. Dunstan, Yiwei W. Sun (School of Physics and Astronomy, Queen Mary University of London)

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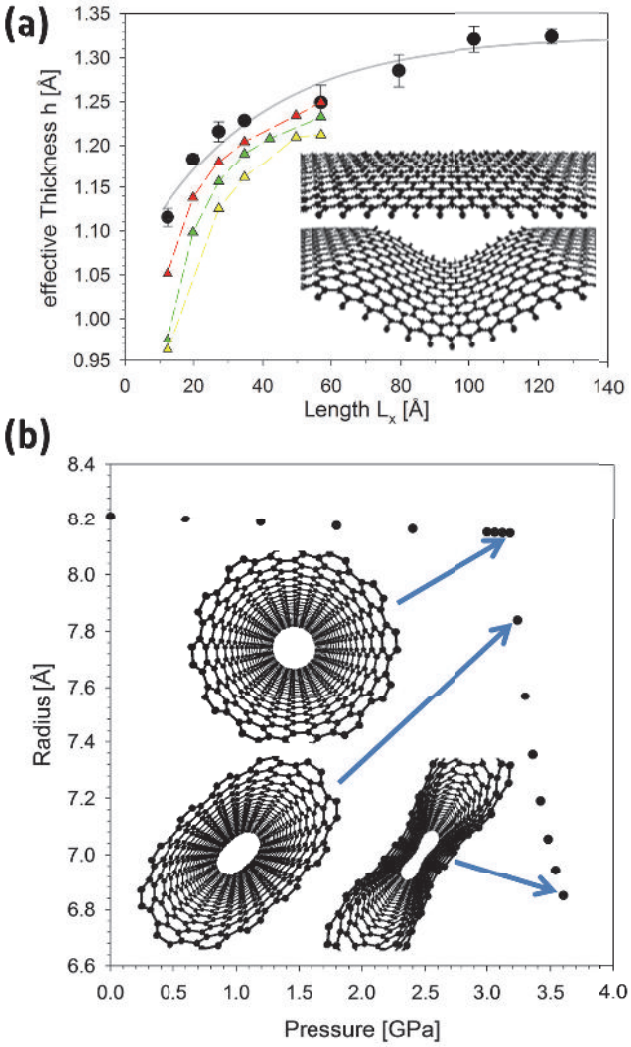

Fig. 4 *(a) The effective thickness of graphene as a function of its size. (b) The pressure induced hard-to-soft transition of nanotubes.*

Structural- & crystalline properties of 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 and diffraction techniques (SAXS, 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. *Semiconductor* nanocrystals can be used as efficient detectors for the infrared in organic 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) The shell's structure in PbS/CdS core/shell nanocrystals affects their photoluminescence

The infrared emission of lead chalcogenide nanocrystals (NCs) can be drastically increased stabilising the core with a hard protective shell [2, 3]. In contrast to a shell growth on top of a core [3], we investigated in this study the CdS-shell growth on PbS NCs driven by Cd for Pb cation exchange [4].

Especially, we studied three different final shell thicknesses of 0.9, 1.5 and 2 nm using three different diameters for the initial PbS NCs of 4.7 nm (small), 6.3 nm (medium) and 8.7 nm (large). The chemical core/shell profile as a function of reaction time is derived from anomalous SAXS (ASAXS) experiments in sub-nanomter resolution measured at the synchrotrons ESRF and HZB-BESSY. The crystal structure of the shell was derived by XRD combined with TEM measurements, respectively. We relate the chemical and structural information to the measured PL intensities of the core/shell NCs.

We reveal the existence of two different crystalline phases, i.e. the metastable *rock salt* and the equilibrium *zinc blende* phase within the chemically pure CdS-shell. The highest improvement in the PL emission was achieved for 0.9 nm shells depicting a large metastable *rock salt* phase fraction matching the crystal structure of the PbS core [4].

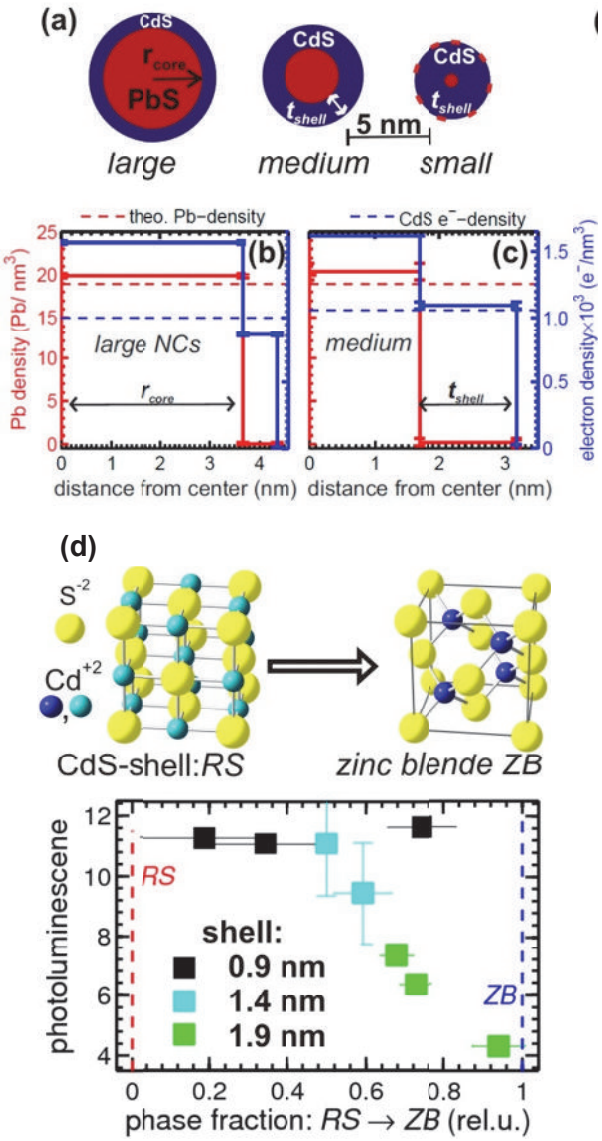

***Fig. 1**: **(a)** Sketch of the investigated PbS/CdS core/shell NCs with three different sizes. **(b)-(c)** Chemical profile of the large and medium sized NCs derived from ASAXS. **(d)** PL intenisty of the core/shell NCs as a function of the shell's crystal structure. The PL is normalised to the shell thickness as well to the total Pb amount within the NCs*

2) In-situ synchrotron studies of colloidal crystallization and the influence of the nanocrystal shape

Colloidal crystals using crystalline nanoparticles (NCs) as building blocks offer the opportunity for designing artificial solids with tailored properties [1]. The assembly of colloidal crystals is not only influenced the by the NC-size, but also by the shape of the individual NC. One reason for the deviation of the spherical shape is the crystallographic facet formation on the NC surface, in order to minimze the total free surface energy. The recently achieved control of the NC syntheses process [1] results in size distributions below 5%. This allows the use of SAXS methods to retrieve the mean shape of a large ensemble of inorganic NCs.

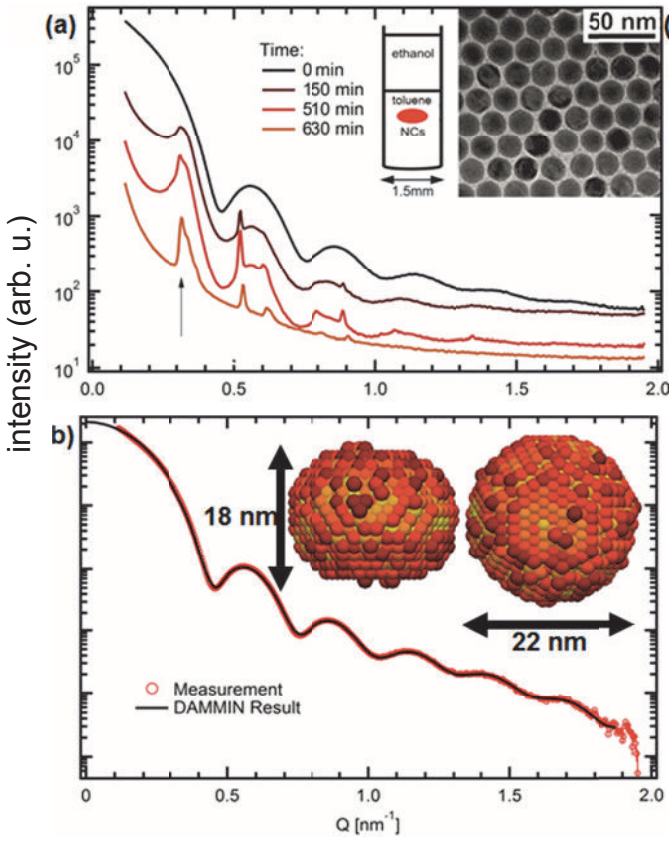

Fig. 2 (a) *Time resolved in situ SAXS patterns of the formation of self-assembled colloidal crystallization of Bi -NCs shown in the inset.* ***(b)*** *SAXS pattern (red spheres) compared to the calculated fit (black line) for the faceted shape using a dummy atom model of arround 1 nm shown in the upper inset. (both measurements were performed at the Austro-SAXS beamline at ELETTRA.)*

We studied by in-situ SAXS/WAXS the template free self-assembled colloidal crystallization by diffusion of a non-solvent into the colloidal dispersion [5]. The SAXS patterns of the NC ensembles were recorded below the NC-solvent/non-solvent interface at the Austro-SAXS beamline at the synchrotron ELETTRA. Hence, we can follow the crystallization process in short time steps as a function of the non-solvent concentration.

Furthermore, we revealed that the 22 nm Bi NCs are nearly monodisperse, but deviate significantly form a spherical shape. A good correspondence between SAXS data and fit was found for an elliptical shape with two main axes of 18 nm and 22 nm (see Fig.1), which could not be detected with previous TEM studies. A nearly perfect fit was achieved by using the ATSAS software package developed originally for the shape retrieval of monodisperse protein structures. The obtained mean shape clearly reveals the facetted NC surface (see Fig. 1b). Only with this derived asymmetric shape we were able to explain the observed super crystal lattice peaks and hence revealed the influence of the NCs' shape on the colloidal lattice formation.

3) Multiferroic semiconductor nanostructures

A further research topic is the growth and characterisation of multiferroic semiconductor structures in cooperation with G. Springholz from the JKU-Linz. $Ge_{1-x}Mn_xTe$ is shown to be a multiferroic semiconductor, exhibiting both ferromagnetic and ferroelectric properties. By ferromagnetic resonance we demonstrate that both types of order are coupled to each other. As a result, magnetic-field-induced ferroelectric polarization reversal is achieved. Switching of the spontaneous electric dipole moment is monitored by changes in the magnetocrystalline anisotropy. This also reveals that the ferroelectric polarization reversal is accompanied by a reorientation of the hard and easy magnetization axes. By tuning the GeMnTe composition, the interplay between ferromagnetism and ferroelectricity can be controlled.

Cooperation:

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H. Amenitsch (ELETTRA, Triest)
A. Hoell (HZB-Berlin, BESSY II)
T.U. Schülli (ESRF, Grenoble)
M. Kovalenko, M. Yarema (ETH, Zürich)

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Biomimetic Materials Research

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The main focus of our research on biomimetic materials was on silica biotemplated by plant materials. Other work was related to SAXS evaluation techniques and to cellulose films. An invited *Feature Article* in *Advanced Functional Materials* summarizes recent progress of our group in this field [1].

1) Biomimetic processing of wood

The structure of wood is a hierarchical one, where parallel microfibrils consisting of parallel cellulose fibrils and hemicelluloses wind helically around the interior lumen of a wood cell. The space between the microfibrils is occupied mainly by lignin. We have already shown that the microfibrils can be replicated in silica [2].
Two of the remaining questions were the actual formation process, and if the cellulose fibrils were also replicated. Therefore the scattering of spruce (*Picea abies*) wood samples which were pre-treated and impregnated with TEOS, was recorded *in-situ* during the heating process.

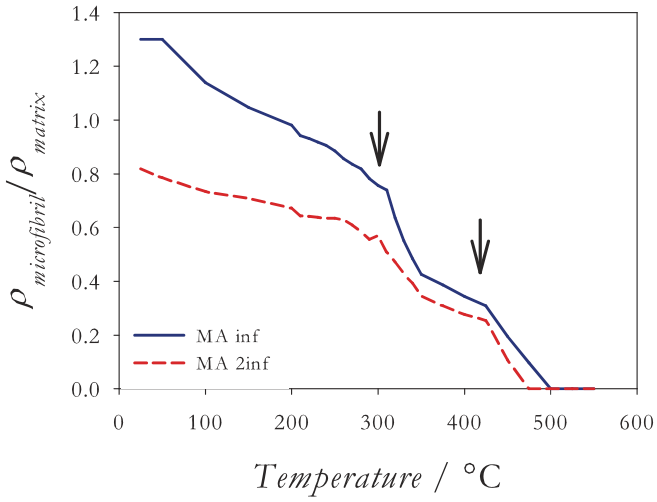

***Fig. 1** Electron density ratio of cellulose fibrils relative to the surrounding material. The arrows indicate decomposition of hemicelluloses and of cellulose.*

The evaluation of the data showed that the replicas are formed stepwise [3]. At about 250-300°C the hemicelluloses disintegrate leaving the organic material of the cellulose fibrils embedded in the silica matrix. At 350-450°C the cellulose decomposes leaving pores where the fibrils used to be (Fig. 1). At the same time this shows that the complete hierarchical structure was replicated since the hemicelluloses template the silica, while the cellulose templates the pores embedded in this silica matrix.

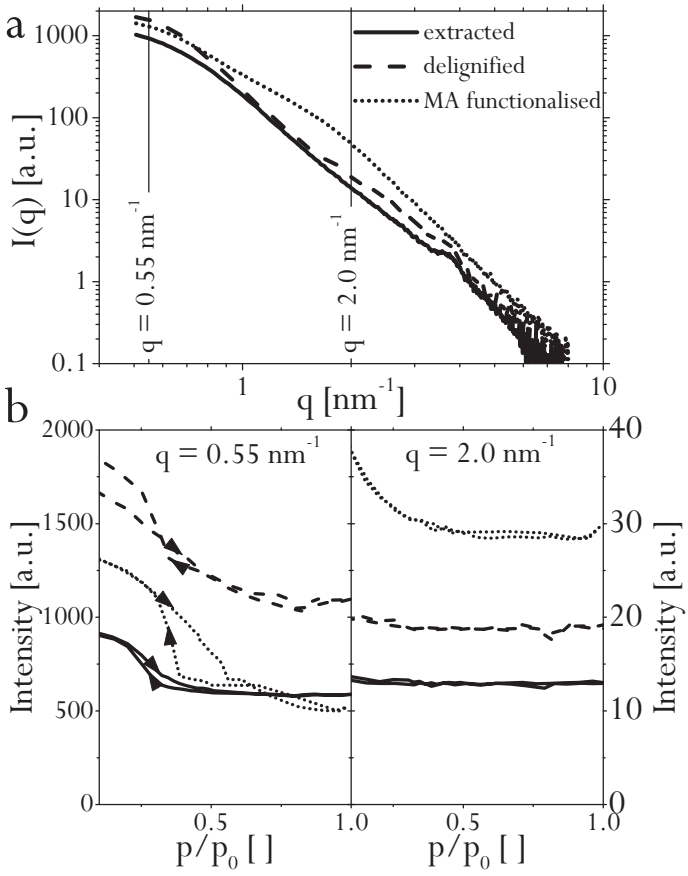

***Fig. 2** SAXS spectra of replica of differently treated wood templates (top) and intensity as a function of n-pentane pressure at constant scattering angles (bottom)*

The pores also influence the mechanical properties of the material leading to a higher toughness of the material due to better energy dissipation by irreversible collapse of the nanopores [4].
The resulting pores are of various sizes. The lumina on the cells result in macropores, the interstices between the microfibrils in mesopores and the cellulose fibrils in micropores. Sorption measurements combined with *in-situ* SAXS measurements showed (Fig. 2) that the mesopores of all replicated samples were similar. The templates that were functionalized with maleic acid anhydride prior to infiltration with tertraethyl-orthosilicate contain also a large number of micropores. These micropores are open ones and can be accessed by gases.

2) Other biological materials

The replication process can be also used for other materials. One of these materials are pine cones. The orientation of the microfibrils in pine (*Pinus nigra*) cones differ greatly within one scale in order to allow for humidity dependent movement [5]. Therefore it is essential to know the spatial arrangement of the fibril orientation and the degree of orientation in native scales.

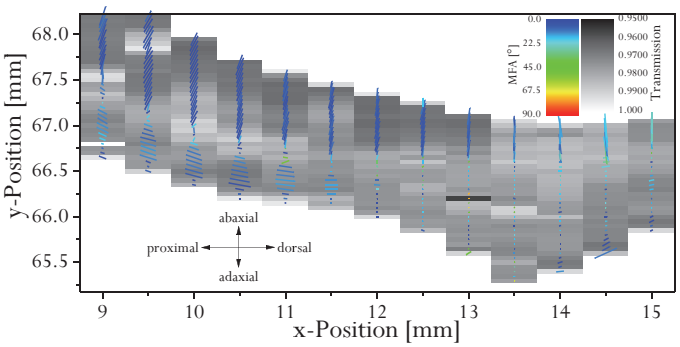

Fig. 3 *x-ray transmission and fibril orientation of a native pine cone scale. The lines indicate the direction of the microfibrils, their length the amount of oriented structures.*

Scanning SAXS measurements of the region, which controls the movement of one scale, show the expected bilayer arrangement (Fig. 3). The microfibrils in the abaxial part are oriented normal to the surface, the ones in the adaxial parallel. The abaxial layer becomes thinner in dorsal direction. Additionally there is a region between proximal and dorsal parts of the adaxial layer, where the structures are hardly oriented. All this is in good agreement with the observed closing of the wet cone due to swelling.

Another plant structure with interesting properties is the pomelo (*Citrus maximus*) peel, since its foamy structure allows for good absorption of mechanical shocks. Such a peel was used as a template[6]. The replica (Fig. 4) is a multiscale ceramic foam, which combines a gradient of size of macropores with nanometer sized pores within the cell walls.

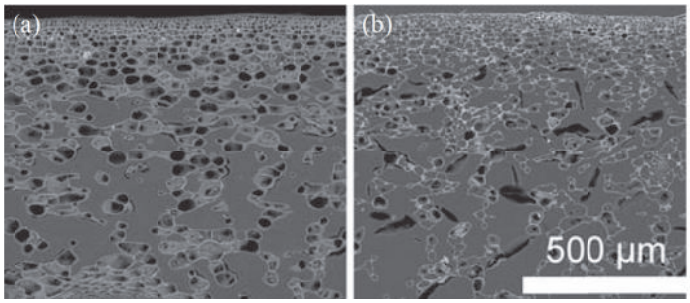

Fig. 4 *Scanning electron micrograph of native pomelo pee (left)l and its silica replica (right)*

3) Other activities

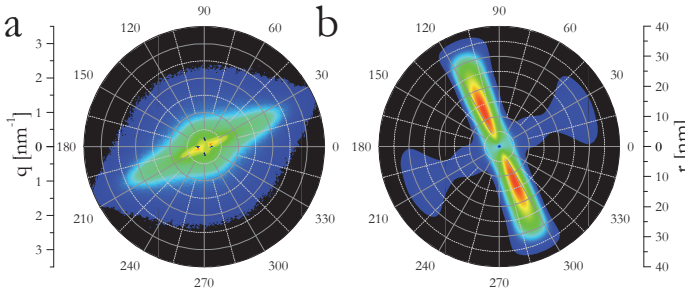

Fig. 5 *Scattering pattern of replicated wood (left) and the corresponding real space function (right)*

The nanostructures in wood show a preferred orientation. This is reflected in scattering patterns, which show a strong streak in the direction normal to the microfibril orientation. The interpretation of the experiments should lead to a real space model. Therefore it can be of advantage to transform the 2D scattering pattern into a real space function for further interpretation.

A two dimensional indirect Fourier transformation [7] technique has been developed. It allows for the computation of such real space functions without loss of information (Fig. 5).

Another activity was on transparent cellulose films containing EuF_3 crystals[8]. It could be shown that the supercritically dried films contain pores in the size range of about 12 nm. The crystals had sizes of about 20 nm and aggregated within the film.

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Cooperation:

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Nanoporous Materials & Physics in Confinement

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The physics of fluids and condensed matter in nano-confinement is a research topic of ongoing interest in our group. This includes the characterization of the nanoporous hosts, the adsorption properties and the phase behavior of the guest molecules, and the mutual interaction between host and guests. Of particular interest within the current reporting period was the deformation of the porous materials due to their interaction with the guest molecules - notably water - during adsorption, condensation, or freezing. As material model systems we employ highly ordered mesoporous silica, consisting of cylindrical pores with diameter 2-10 nm with narrow size distribution which are arranged on a two-dimensional pore lattice. This specific arrangement allows employing small-angle X-ray and neutron diffraction techniques for the in-situ determination of pore lattice strains as a function of thermodynamic variables such as pressure or temperature. Within a project funded by the Federal Government of Styria, we have extended this research towards potential applications of sorption induced deformation for medical sensors.

1) Water freezing in confinement

Besides the influence of confinement on water properties [1-3], the mechanical response of the porous framework on the freezing and melting of water was studied in detail [4, 5]. This effect is of importance for many phenomena of everyday life, such as for instance for frost damage of roads. Using in-situ X-ray diffraction, the pore lattice strain of water filled pores of different diameter was determined as a function of temperature First, due to the Gibbs-Thomson effect, the freezing/melting transition is shifted to lower temperatures, the smaller the pores are. Second, around the melting point the strain shows a strong non-monotonous change with temperature (Fig. 1, middle part), which cannot simply be attributed to the thermal expansion of water and ice. Using classical concepts of thermodynamics, this effect can be explained by the fact that a liquid, wetting the pore wall material in equilibrium with its solid phase, will be thermodynamically favored in confinement. Formally, this leads to a generalized (negative) Laplace pressure in the pores, which in turn leads to the observed compressive deformation of the pore lattice. Fig. 1 shows the close analogy between pore lattice deformations due to capillary condensation (gas-liquid transition) governed by the Kelvin Equation, and due to melting (solid-liquid transition) governed by the Gibbs-Thomson equation. As a practical aspect, such experiments allow deducing a stiffness parameter of the nanoporous material.

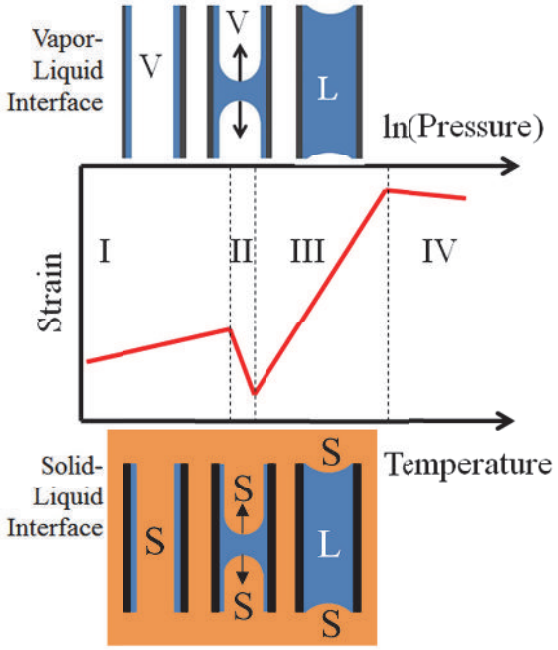

Figure 1: Scheme of the analogy between the vapor-liquid (top) and the solid-liquid (bottom) phase transition mechanism of water in cylindrical mesopores, leading to the experimentally observed pore lattice strain in regions II and III (middle). The silica walls (dark grey) are in contact with the liquid water phase (blue) and with the water vapor (white), or the solid ice phase (orange). (Adapted from [4]).

2) Sorption induced strains in mesoporous films

Generally, the adsorption of any species on the pore walls will lead to a change of the surface/interface energy of the solid, which is associated with a surface stress. This leads to a bulk stress in the solid, which in turn leads to sorption induced deformation of the porous material. One of the possible applications of sorption induced deformation is towards sensor or actuator materials and devices. Fig. 2 shows the principle of a possible device based on a simple bilayer structure, which should bend upon adsorption of molecules due to different expansion/contraction of the two layers. The goal of our research here was to test this hypothesis by fabricating micro bending-bars and to investigate their sorption induced deformation. In a first step, ordered mesoporous silica films were prepared on silicon substrates by applying known procedures of evaporation-induced self-assembly, and their deformation behavior upon water adsorption was studied [6]. Fig. 3a shows the GISAXS (Grazing-Incidence Small-Angle X-ray Scattering) pattern of a spin-coated film of 100 nm thickness. This pattern can be attributed to elongated pores with elliptical cross-section on a centered 2D-rectangular pore lattice. The point-like pattern indicates that the pores are perfectly oriented with respect to the film surface, the long pore axis lying preferentially within the plane of the film.

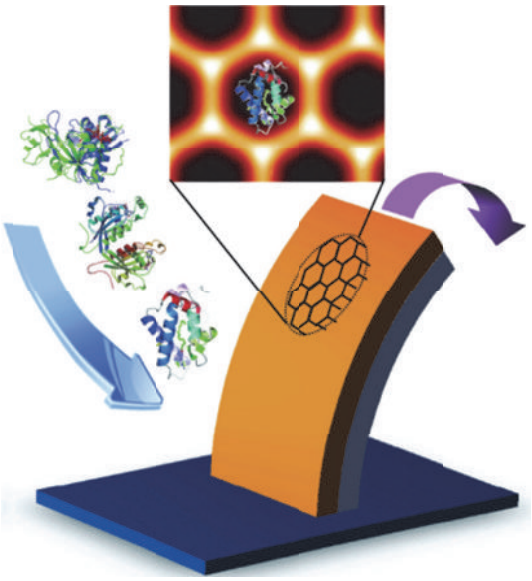

Figure 2: Scheme of a bilayer actuator which bends upon the adsorption of proteins due to sorption induced deformation of a mesoporous.

Water adsorption/desorption in differently prepared films was investigated in-situ using a custom built humidity chamber at the Austrian SAXS beamline at the synchrotron radiation source ELETTRA in Trieste, Italy. For the first time, both, out-of-plane and in-plane strains in the films as a function of relative humidity could be determined quantitatively from the GISAXS patterns (Fig. 3b). The results show a strong out-of-plane strain upon capillary condensation, but a much smaller in-plane strain for a thin (100 nm) film, as expected for a homogeneous thin film tightly bonded to a rigid substrate. The situation was however different for a thick (>500 nm) film, where considerable in-plane strains were observed.
Besides the mesoporous films on silicon wafers, we have also managed to prepare films on one side of AFM cantilevers. This was achieved by hydrophobisation of one side of the cantilever using self-assembled monolayers, followed by dip coating and EISA of the silica precursor on the hydrophilic side of the cantilever only. Preliminary experiments in a humidity controlled AFM (Teichert group) show a clear cantilever bending upon change of the humidity, demonstrating the fundamental working principle of the device.

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Cooperation:
1) Dirk Wallacher (Helmholtzzentrum Berlin).
2) Christian Teichert, Christian Ganser (MU Leoben); Heinz Amenitsch, Benedetta Marmiroli, Barbara Sartori, Fernando Cacho-Nerin (TU Graz and SAXS beamline, ELETTRA Trieste); Annelie Weinberg, Lisa Martinelli (Med. Univ. Graz).

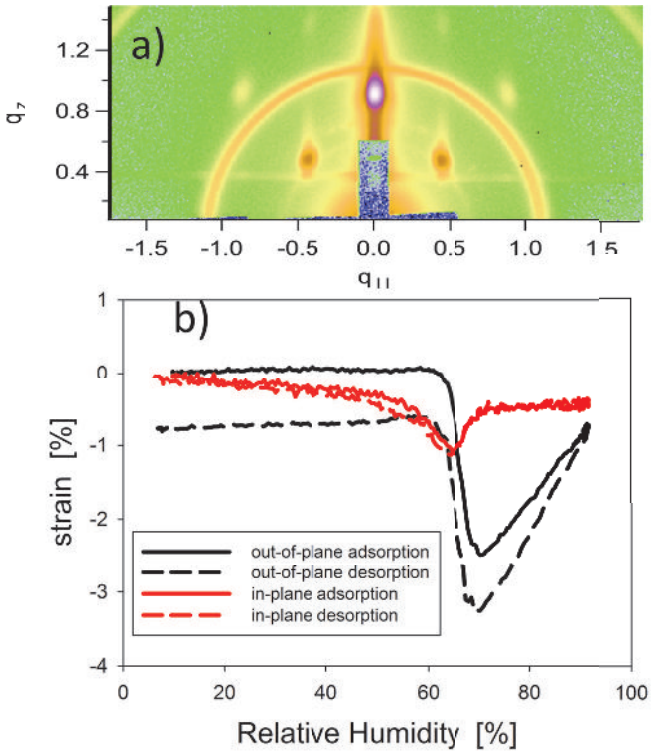

Figure 3: a) GISAXS pattern of a 100 nm mesoporous silica film prepared by spin-coating. The sharp peaks indicate a 2D centered quadratic lattice (a = 9.65 nm) of cylinder pores with elliptically deformed cross section. The continuous circular ring is the first order powder ring from an internal standard sample. b) Pore lattice strain as a function of relative humidity. (Figure adapted from [6]).

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Supercapacitors - Ions in Confined Geometry

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Supercapacitors or Electrical Double-layer Capacitors (EDLCs) are devices used for efficient energy storage with high power density. If two inert electrodes are immersed into a liquid electrolyte and a voltage is applied an electrical double-layer is formed at the electrode-electrolyte interface. The opposed charge of ions and electrons reveals capacitive behaviour. In contrast to batteries the energy is predominantly stored electrostatically and not electrochemically. Modern electrode materials such as activated carbons or carbide-derived carbons exhibit specific surface areas up to 2000 m^2/g, leading to capacities exceeding 100 F/g. Since the average pore diameter in such materials is typically below 1nm, the formation of a double-layer according to classical models is not easily possible. It was found that ions can penetrate into pores smaller than their solvated ion size losing parts of their solvation shell [1]. The arrangement and the transport of ions in such pores as a function of electrical potential is still a matter of debate, and is the major motivation for our work in this field.

1) Ion transport in microporous carbon based supercapacitors

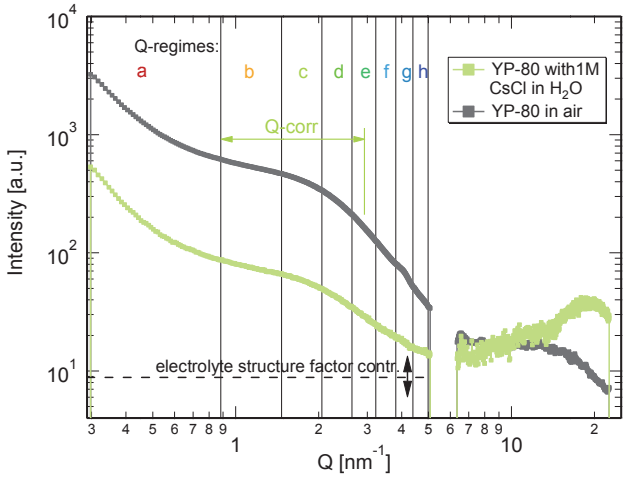

Fig. 1 *SAXS and WAXS intensity of the dry activated carbon YP-80 (grey) and the carbon infiltrated with electrolyte (green). The indicated Q-regimes are necessary for the further data analysis.*

Small- and wide-angle X-ray scattering (SAXS/ WAXS) patterns of an activated carbon are shown in Fig. 1. The sample infiltrated with 1M CsCl aqueous electrolyte show a similar scattering curve in the SAXS regime. In the WAXS regime the structure- factor of the liquid electrolyte overlays the contribution of the carbon structure factor.
A specially designed *in-situ* cell enabled the study of the electrolyte-wetted carbon electrode in model supercapacitors while applying an electrical voltage. The dependence of the SAXS and WAXS intensity on the applied voltage cycling (Fig. 2) was measured at the Austrian SAXS beamline at the synchrotron radiation source ELETTRA in Trieste.

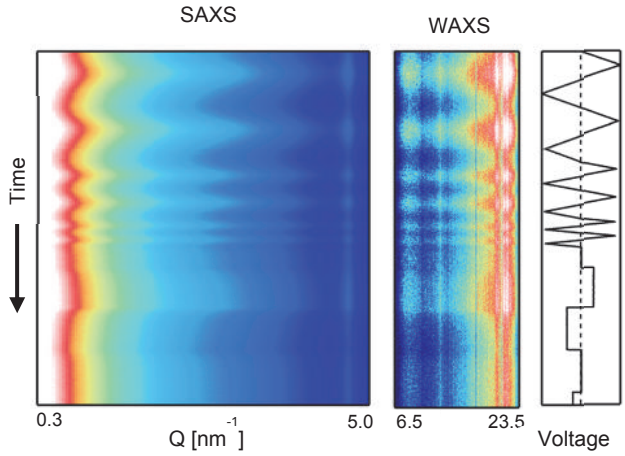

Fig. 2 *The as-measured SAXS (left) and WAXS (middle) intensity is shown in a colour coded scale as a function the applied voltage signal (right).*

First, the electrolyte structure factor contribution is evaluated and subtracted using a simple model. Then, integral parameters are calculated for specific regimes of the scattering vector length Q in the scattering curves (Fig. 1). While the integrated intensity usually corresponds to a change in the average scattering contrast, the correlation length - defined by the ratio of the first to the second moment of the scattering curve - is sensitive to structural changes within a certain length scale. The SAXS intensity covers mainly changes within the micro- and mesopores (Nanometer-regime). In contrast, the X-ray transmission signal, which was simultaneously measured using a photodiode, covers electron density changes within all pores (micro-, meso- and macropores). All these parameters are shown in Fig. 3 as a function of the applied electrical potential during two CV cycles.
The change in the transmission signal proves the change of the overall cation and anion concentration within the irradiated volume of the carbon electrode. Hence a macroscopic ion transport from one electrode to the other takes place as expected. Fig. 3b shows also that there is a clear “phase-shift” of the transmission signal with respect to the voltage signal. This shift enables ion transport to be analysed in more detail. In particular, the small size of the X-ray beam (1x1mm) enables a measurement on different spots on the electrode within an about 10 mm diameter hole in the model device. A local dependence of the time-constants of the ion-concentration during CV cycling was found, depending on the distance the ions have to travel from one electrode to the other [2].

2) Pore expansion and ion concentration change

Beside the study of the ion transport on different hierarchical levels, other phenomena like a mechanical response of the carbon electrode on ion electrosorption within confinement was found [2]. It is well known from literature that applying a voltage to the highly porous electrode can lead to its macroscopic expansion. This effect is often attributed to an increased electrolyte

pressure within the smallest pores [3] (<2nm) due to increased ion concentration. In other studies the expansion or contraction was exclusively explained by a change in the carbon interfacial energy due to the change of the binding situation for surface atoms when inserting electrons. [4]

In general the change in the integrated intensity (Fig. 3a) is caused by the change of the electron density contrast between pores and carbon matrix. If Cs^+ ions with large scattering cross-section enter the pores at negative potential, the SAXS intensity is expected to decrease. This is the case at large values of Q, but additionally an intensity increase at small Q-values is observed at negative voltages (see Fig. 3a). By fitting the SAXS curves with the well-known Debye-Anderson-Brumberger model, it was shown in [2] that this effect can be understood by the swelling of the electrode, which leads to an increase of the intensity particularly at intermediate and low Q-values. The swelling is directly observed in the SAXS correlation length in Fig. 3c, shown together with the macroscopic strain of the electrode measured with dilatometry by our partners at the INM. This provides an independent evidence that the correlation length measured with SAXS has its origin in the change of the pore size. At negative voltages the pores expand while at positive potentials the pores basically shrink with respect to the 0V size, before they slightly expand around the voltage maximum. The asymmetric swelling behaviour for positive and negative ions suggests at least two different physical mechanisms being responsible for the pore expansion behaviour. A detailed analysis of the transmission and the electrical current signals allows the calculation of the absolute ion concentration change within the pores in dependence on the applied voltage. The total ion concentration was found to be constant for all potentials, while only the cation/anion ratio changes. Hence a direct correlation of the total ion concentration to the pore expansion was not found. Further systematic work - desirably on carbons with narrower size distribution - is required to better understand this interesting but hitherto unexplained swelling behaviour.

In conclusion, this study demonstrates for the first time the possibility of studying ion transport and pore expansion in highly disordered activated carbons by analysing integrated SAXS parameters for defined Q-regions during in-situ voltage cycling in model supercapacitors.

Cooperation:

Volker Presser, Daniel Weingarth, Emilie Perre, Institut für Neue Materialien (INM) Saarbrücken.
Heinz Amenitsch, TU Graz and ELETTRA Trieste.

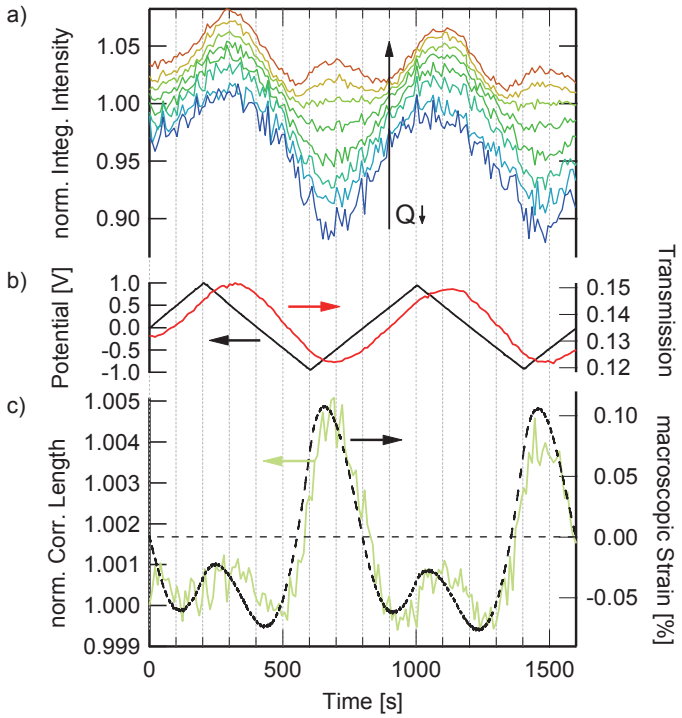

Fig. 3 *a): Integrated intensity as a function of time (or applied voltage signal) for different Q-regimes. b) Applied voltage signal (black) together with the measured X-ray transmission signal (red). c) SAXS correlation length (green) for the Q-regime "Q-corr" and macroscopic electrode strain measured by dilatometry (dashed black).*

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Surface Physics & Scanning Probe Microscopy

Cellulose based materials

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Cellulose is an abundant biopolymer present in modern daily life as paper, textiles, and hygiene products.
The motivation to study different cellulose materials is to gain insight into fiber-fiber bonds in paper. For that reason, model systems like cellulose films and regenerated cellulose fibers were employed. Also, single kraft pulp fibers as well as bonds between them were investigated. The model systems allow to isolate single contributions to bond strength such as swelling or Coulomb interactions and to test their influence on bonding. By testing the more complicated pulp fibers and their fiber-fiber bonds, additional mechanisms such as interlocking of fibrils between two fibers and the swelling behavior of the whole fiber are revealed.
This work was carried out within 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) Mechanical properties of cellulosic materials

By using diamond AFM tips as an indenter, mechanical properties of various cellulose materials can be probed on the nanometer scale [1,2]. This so-called AFM based nanoindentation (AFM-NI) yields the hardness and the reduced modulus, which correspond to a material’s yield strength and elastic modulus, respectively.
First, amorphous cellulose model films were investigated under ambient conditions (see Fig. 1) and in the fully swollen state. The effect of swelling on the mechanical properties could be influenced by adding salt to the swelling solution or spin-coating a layer of xylan to the cellulose film.
Then, the method was applied to single pulp fibers at relative humidities between 6% and 80% as well as in the fully swollen state. A continuous reduction by two orders of magnitude between dry and wet fibers was observed.
This large decrease of hardness and reduced modulus in water facilitates the formation of bonds with a very high area of molecular contact. During the drying process of paper, capillary bridges will form between two fibers and pull them into close contact [3].

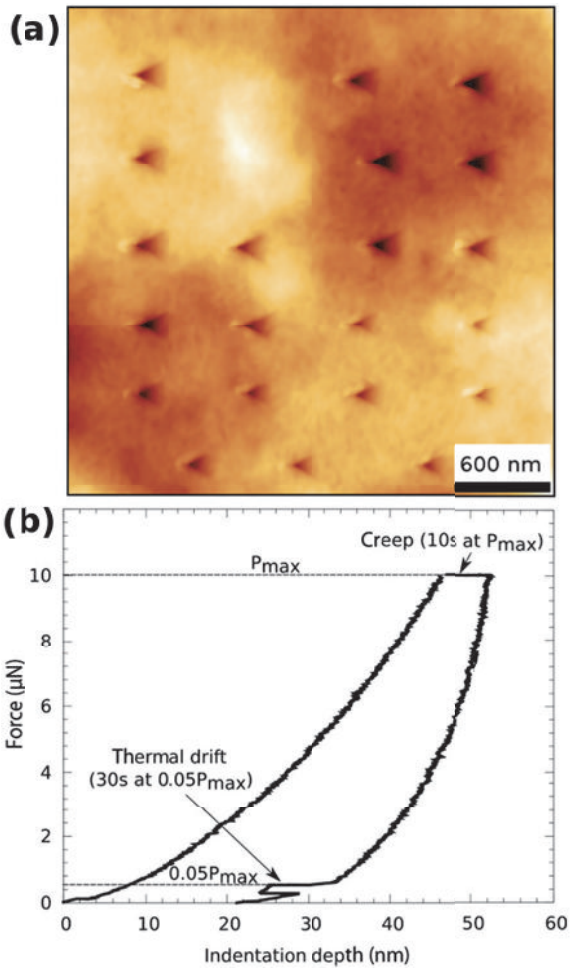

Fig. 1 (a) AFM topography image of an amorphous cellulose film with indents and (b) exemplary force-vs-indentation depth plot recorded on this surface. (From [1].)

2) Water absorption studies of cellulose fibers

Regenerated cellulose fibers are used in textiles and hygiene products, these are two applications where the ability to absorb water is of crucial importance.
In order to find out, why two nominally identical viscose fiber samples had different absorption properties, AFM investigations were carried out on the fiber surfaces. It was found that the roughness parameters were similar on both samples and surface trenches were present. A closer investigation of the trenches, revealed that fibers with a high ability to absorb water exhibit a low density of trenches and vice versa.
Also, a direct approach to study water uptake of regenerated fibers was chosen. In collaboration with the Nanomaterials & Scattering Group (Roland Morak and Oskar Paris), viscose fibers with different cross-sections were compared to never-dried, bleached softwood kraft pulp fibers using an adsorption microbalance. The investigations were carried out with a low and a high amount of fibers, which were 20 mg and 100 - 200 mg, respectively. The low mass series is most likely to correspond to single fiber properties and yielded no significant difference between the samples. On the other hand, with the high mass series, the network properties of the samples are measured. Here, a difference was found, implying that the fiber surfaces which interact with each other play a larger role than the fiber's bulk properties.

3) Xylan precipitates on cellulose model films

Amorphous cellulose films can be used to study the interaction of two cellulose surfaces with each other, by bonding them together and measure the force needed to separate them again. To simulate the presence of hemicelluloses – as in pulp fibers – xylan was precipitated on cellulose films. By using functionalized AFM tips (OH and CH_3) in tapping mode, xylan could be identified on the surface by a distinct phase contrast. Additionally, the adhesion force of the tips to the surface was recorded by force mapping. In Fig. 2, the topography and its corresponding force map is presented. Both, OH and CH_3 functionalizations, exhibit a lower adhesion force to xylan than to cellulose.

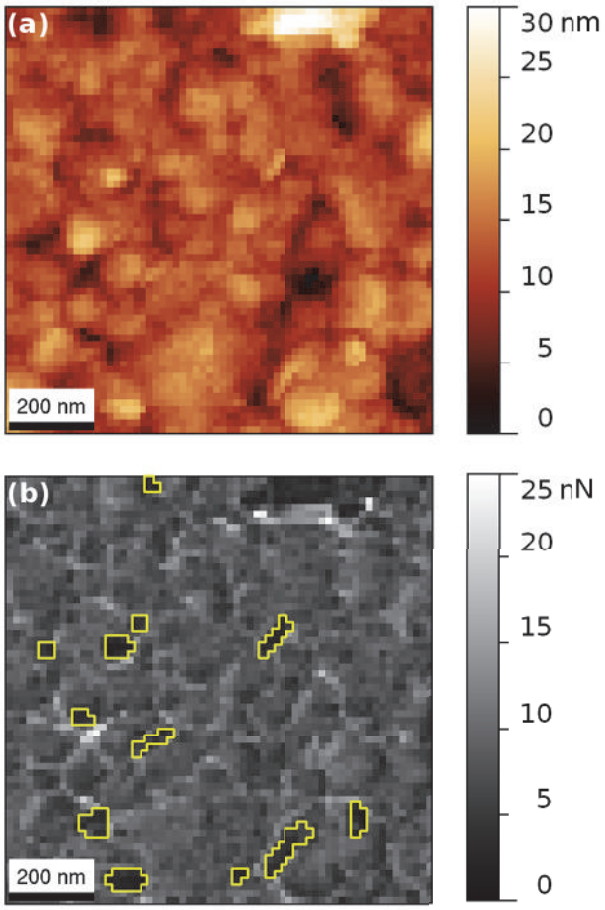

Fig. 2 Topography (a) and the corresponding adhesion force map (b) of a cellulose model film with xylan precipitates, recorded with an OH-functionalized tip. Regions with lower adhesion force represent xylan aggregates and are encircled with yellow lines in (b).

With the combination of phase imaging and force maps, xylan precipitates with a typical diameter of 25 nm were successfully located on the cellulose surfaces [4].

4) Mechanical interlocking in fiber-fiber bonds

By using an approach to test fiber-fiber bonds with an AFM based method [5,6], the effect of refining on bond strength was studied. In the process of refining, pulp fibers are beaten mechanically which increases a fiber's surface area and its conformability.
In this AFM based fiber-fiber bond strength test, the force is applied by an AFM cantilever and the force exerted on the bond is measured by detecting the cantilever's deflections [5]. Unrefined and refined fiber-fiber bonds were tested and force-vs-distance (F-x) curves were recorded. In Fig. 3, typical F-x curves of a refined and an unrefined bond are displayed. The F-x curve of the refined bond features several jumps, whereas the refined curve is completely smooth. It is obvious that the refined bond absorbs much more energy during the rupture than the unrefined bond. The most likely explanation is that due to refining, cellulose fibrils are freed and are dangling from the surface. During bond formation, they interlock with each other – in a similar manner as a velcro fastener – leading to a bonding mechanism, which is not present in unrefined bonds [6].

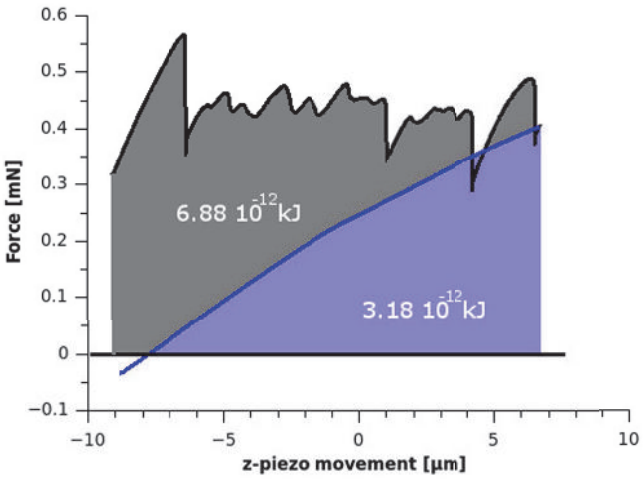

Fig. 3 Force-vs-distance plot of a refined (grey) and an unrefined (blue) fiber-fiber bond. The areas under the curves represent energies absorbed by the bonds during rupture. (From [6].)

Cooperation:

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Physics of Interfaces and Nanomaterials, University of Twente);

Walter Roggenstein, Ingo Bernt (Kelheim Fibres GmbH);

Leo Arpa, Franz J. Schmied (Mondi Frantschach).

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Surface Physics & Scanning Probe Microscopy

Growth of small organic molecules on graphene

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Besides its exotic electronic behavior, graphene (Gr) has a variety of benchmarking physical properties like high mechanical strength and almost 98 % transparency in the entire visual spectral range. The latter makes it an ideal candidate for a transparent electrode to replace indium tin oxide (ITO) in light emitting diodes, solar cells, and touch screens. To explore this hypothesis, growth experiments of small organic molecules on graphene are essential. For the applications mentioned above, the molecules should orient on the substrate in a lying fashion. Employing low-energy electron microscopy, we demonstrated previously that para-hexaphenyl (6P) indeed grows on Ir(111) supported graphene at 240 K with this orientation in a layer-by layer mode [1]. The unavoidable wrinkles in epitaxial graphene act as nucleation centers [2]. At room temperature, crystalline 6P needles - still composed of lying molecules - are observed [3].
Here, we investigate temperature dependent growth morphologies of 6P on wrinkle-free, exfoliated graphene that has been transferred on SiO_2 films. The growth has been performed by hot-wall epitaxy (HWE) under high vacuum in the temperature range from 280 K – 423 K. On silicon oxide, 6P exclusively forms islands composed of standing molecules, whereas on the graphene flakes preferentially needles are observed which grow longer at elevated temperatures and form networks with discrete needle orientations [4]. This is demonstrated by atomic-force microscopy (AFM) in Fig. 1 for the case of 363 K.

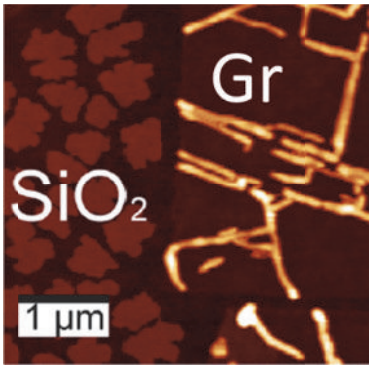

Fig. 4 *AFM topography image of HWE grown 6P on SiO_2 and exfoliated single layer graphene. (z-scale: 10 nm; from [4].)*

Further, it has been found that with increasing temperature more 6P is observed on graphene than on SiO_2 (Fig. 2). This behavior is explained by a reduced sticking of 6P on SiO_2 whereas the molecules still bind to graphene due to π stacking [4].

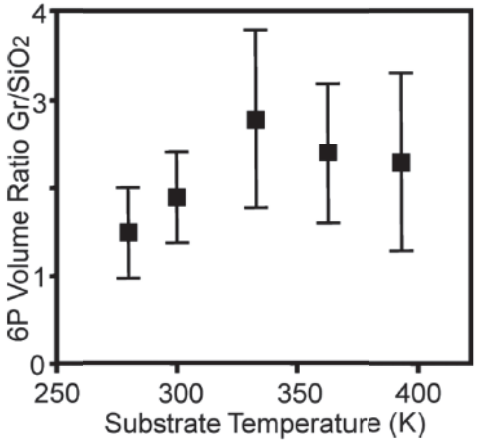

Fig. 5 *Ratio of deposited 6P volumes on Gr and SiO_2 as a function of substrate temperature (From [3]).*

The exfoliated Gr samples exhibit not only single layers of graphene but also double layers of Graphene (DLG) up to a few layers allowing to study 6P growth morphologies as a function of graphene thickness [5]. Fig. 3 shows an AFM image of HWE grown 6P on exfoliated graphene with different layer numbers. One can clearly see that the average needle length decreases with increasing number of Gr layers whereas the needle height increases. This is addressed to a tendency of dewetting for 6P on more graphite like substrates [5]. Fig. 4 presents an illustration of this situtation.

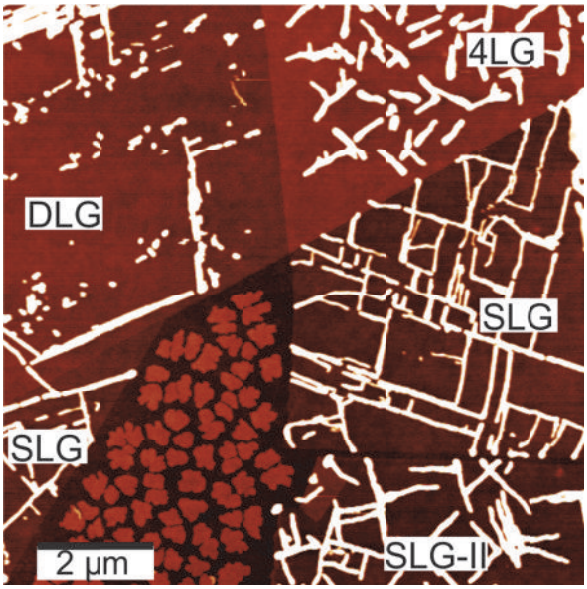

Fig. 3 *10 µm x 10 µm AFM topography image of HWE grown 6P at 363 K. (z-scale: 10 nm), adapted from [5]. Besides SiO_2, single layer (SLG), double layer (DLG), and four layer thick graphene areas are visible.*

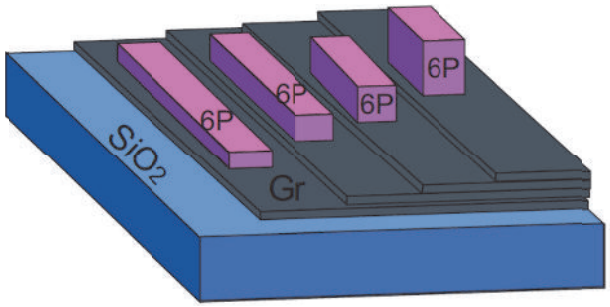

Fig. 4 *Sketch of 6P morphology evolution as a function graphene thickness in monolayers.*

The tendency of 6P to form on graphene at room temperature crystalline needles is recently used by us to probe the cleanliness of chemical vapor deposited (CVD) and subsequently by polymethylmetacrylate (PMMA) transferred graphene.

Further, we have demonstrated the mechanical robustness of graphene [6] by AFM based dynamic plowing lithography (DPL) where the tip of a vibrating AFM cantilever is used to cut graphene. Fig. 5 shows an AFM image of a single layer graphene flake after 7 cuts performed from the bottom to the top by DPL. The applied effective forces increase from about 20 μN to 60 μN. While for the cutting experiments with the two lowest forces no change in topography is found, experiment number 3 resulted in a 1 nm deep and 40 nm wide trench. This has been interpreted as an indentation of the underlying silicon oxide and just a straining of the covering Gr [6]. For higher applied forces (40 μN – 60 μN), the Gr is indeed cut and rolled up to the top. Employing conductive AFM and Kelvin probe force microscopy we detected for ring-like nanostructures cut out by DPL from single layer graphene flakes in which cases the cuts where complete and no electrical connection to the surrounding flake were left. It should be noted that the required forces for completely ripping Gr are only one order of magnitude smaller than forces between single fibers in packaging paper.

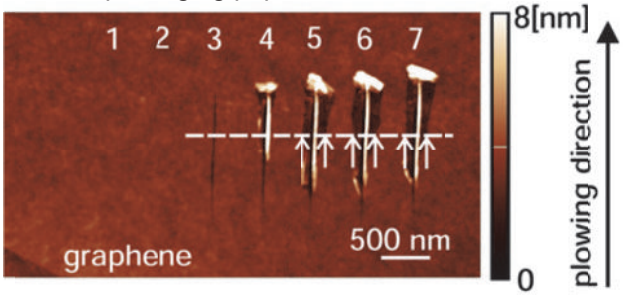

Fig. 5 *AFM morphology analysis of 7 DLP experiments on exfoliated Gr on SiO_2. The applied forces increase from about 20 μN (#1) to 60 μN (7). In cuts 4 - 7, the* vertical white lines next to the trenches in *SiO_2 are plowed silicon oxide bulges. The white arrows point to the resulting graphene edges.*

Cooperation:

Gregor Hlawacek, Fawad Khokhar, Raoul van Gastl, Bene Poelsema, and Harold Zandvliet, Physics of Interfaces and Nanomaterials, MESA+ Institute for Nanotechnology, University of Twente, Enschede, NL, (LEEM);

Borislav Vasić, Uroš Ralević, and Radoš Gajić, Institute of Physics, University of Belgrade, Belgrade, Serbia, (exfoliated graphene + DPL);

Bernhard Bayer, Piran Kidambi, Andrea Cabrero-Vilatela, and Stefan Hofmann, Dept. of Engineering, University of Cambridge, UK, (CVD graphene).

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Triboelectric charge behavior studied by Kelvin Probe Force Microscopy

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Electrostatic charging of surfaces is successfully applied in triboelectrostatic separation of mineral particles. Particles charged upon contact with each other are separated in an electric field (Fig. 1) depending on the sign and amount of the surface charge. However, the knowledge about the charge exchange during the insulator-insulator contact is still limited. A list of factors which should be taken under consideration during building a model of the triboelectrostatic separation was compiled in [1].

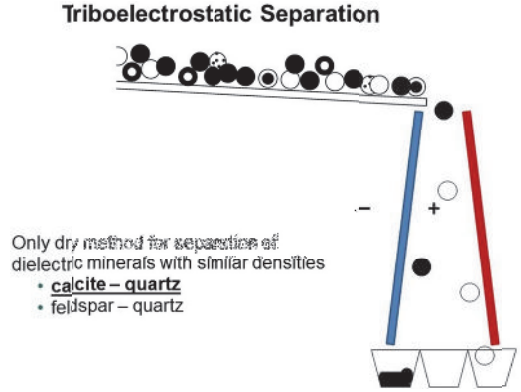

Fig. 6 *Scheme of the triboelectrostatic separation in the free fall separator.*

Here, we study the electric charging of well-defined dielectric surfaces (quartz and calcite single crystals) upon contact with conventional atomic force microscopy (AFM) probes and with micrometer sized single calcite particles glued to the end AFM cantilevers (modified AFM tip). We examined the effect of different contact types like static contact, point charging, and rubbing, on the charging. Contact mode AFM was applied for charging, whereas Kelvin probe force microscopy (KPFM) was employed for determining topography and local surface potential of the sample before and after charging [2]. This methodology allowed us to investigate – at the submicrometer scale – the influence of parameters such as contact force, time of contact and contact with a charged/uncharged object on charging. Decay of the introduced charge over time was also examined. KPFM measurements were performed in amplitude mode using a two-pass technique.
This work was carried out in collaboration with the Chair of Mineral Processing, Department of Mineral Resources and Petroleum Engineering, Montan-universitaet Leoben under the coordination of Prof. Helmut Flachberger.

1) Contact charging

Contact charging is related to two aspects: firstly, the difference between the work functions of the materials of the sample surface and the AFM probe, and secondly, the local electronic modification of the surface under study caused by the appearance/ introduction of new electronic surface states and the structural rearrangement of atoms in the surface near region (stress, material, and ion transport) [3]. Additionally, the work function value can locally vary by the presence of defects, absorbents, and mechanical stresses on the surface. Moreover, the effect of different charging methods, i.e., from weak single perpendicular contact to complex abrasive contacts of two bodies can have influence on the charging mechanism.
Three methods of localized charging were used for the insulating surface (Fig. 2): rubbing, static charging, and a matrix of static charging. Rubbing simulates tribocharging, whereas static charging and the matrix of static charging simulate single-contact charging and multi-apex charging, respectively.

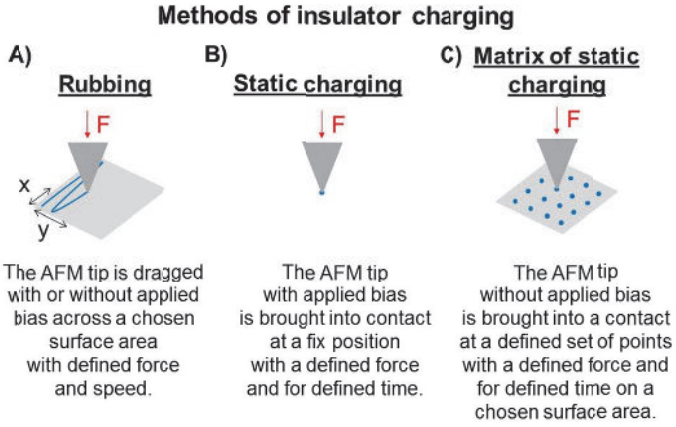

Fig. 2 *Scheme of three methods of charging insulating monocrystals using commercial AFM tips: (A) rubbing, (B) static charging, and (C) matrix of static charging*. (From [2]).

The charged features are observed for each of the all three methods of charging insulating surfaces. Fig. 3 shows a set of 10×10 µm^2 KPFM images of a calcite (100) single crystal surface after charging by the three different methods.
Rubbing (Fig. 3A) caused a change of the surface potential of the rubbed area changed by about 1.5 – 2.0 V and of the surrounding area by 0.8 – 1.0 V. Moreover, charging by rubbing resulted in wear induced changes on the sample surface, especially for high contact forces.

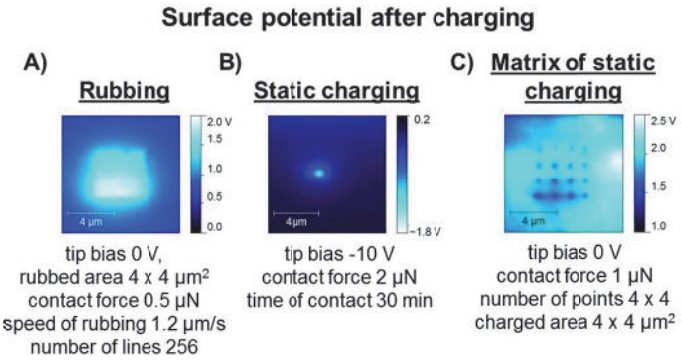

Fig. 3 *KPFM measurements showing results of three methods of charging. 10×10 µm² images illustrate the surface potential of $CaCO_3$ (100) surface after charging: (A) charging by rubbing; (B) static charging; (C) matrix of static charging.*

For a single contact event, change in surface potential was detectable only when an additional bias of ± 10 V was applied to the tip. Static charging with a tip bias of –10 V (Fig. 3B) resulted in a drop of the surface potential by about –0.8 V. In all static charging experiments, the area with resulting change in the surface potential is much larger than the contact area. The effective contact area can be estimated to be just 300 nm² [4], whereas the area with a change in surface potential is in the µm² range. The reason for this observation may be triple. First, introduced charges spread from the point of contact to the surroundings. Second, mechanical stress in the point of contact causes temporally local changes in energetic structures which is preserved and spread by absorbents present on the surface. Third, KPFM detects a weighted average of the sample surface potential [5]. Hence, the potential values obtained from small areas deviate significantly from the true value. Static charging simulates contact charging with a single object or nanoasperity. On the other hand, matrix of static charging simulates simultaneous contact charging with many nanoasperities. A 4×4 point matrix of static charging performed on an area of 4×4 µm², presented in Fig. 3C, resulted in changes of the surface potential by maximum -0.8 V in the charged points, the topography remained unaltered. Increasing number of contacts up to a 32x32 matrix showed a continuous surface potential change within charged area.

2) Contact force / influence of environment / contact with a charged object

Different environmental conditions (temperature, humidity) and experimental parameters (contact force, speed and time, bias, etc.) were investigated.
All experiments showed significant changes in the surface potential due to charging. The common observations are as follow:

- the charged area is much larger than the expected contact area after static contact;
- contact charging becomes more effective with increasing contact force
- the efficiency of the charge transfer decreases for a contact force > 10 µN; complex bipolar surface potential distributions occur; strong changes in the topography are observed;
- both positively and negatively charged areas can be generated on the surface depending on the applied bias polarity during charging;
- asymmetrical behavior of positively and negatively charged areas;
- earlier introduced charge does not influence the value of the surface potential caused by next charging with opposite bias;
- the charges can accumulate during consecutive charging or reach a saturation level (Fig. 4);
- the surface potential is inhomogeneous within the charged area (for rubbing and matrix of static charging);
- the charging behavior significantly differs from sample-to-sample and from place-to-place on the same sample.

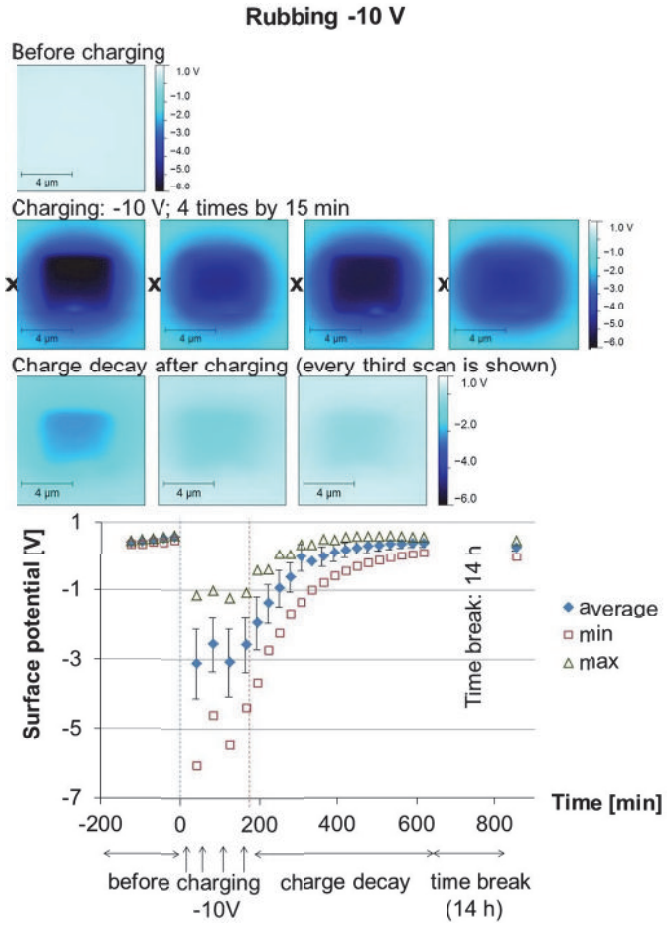

Fig. 4 *KPFM measurements presenting the surface potential distribution for the $CaCO_3$ (100) surface after repeated rubbing on an area of 4×4 µm² with a force of 3 µN and a bias –10 V. Crosses (x) between KPFM images indicate charging events.*
Corresponding curves of surface potential development and decay with time are also shown. Maximum, minimum, and average values of the surface potential collected from an area of 10×10 µm². (From [2]).

3) Charge decay

Typical results for repeated rubbing with applied bias (-10 V) are shown in Fig. 4 together with an analysis of the long-term charge evolution. Here, the charged area is likely to be saturated right after the first charging. Fig. 4 reveals also a decay of the surface potential over time, observed after termination of the charging. The decay time is relatively long, takes tens of hours, and the surface potential changes quasi-exponentially. Moreover, the surface potential introduced during static charging initially decreases much faster than the one caused by the rubbing experiments. The residual charge remains on the surface even for a few days. However, it vanishes after heating the sample up to 100 °C. This might indicate that the charges are partially trapped in stable trap states [3]. The presence of the trap states can be correlated to the local fluctuation of chemical composition at the sample surface, water layer present on the surface, or mechanical deformation caused by the AFM tip. The decay process involves both, discharge due to ions in the ambient environment and the diffusion of surface charges to adjacent areas (decreasing and broadening of surface potential peaks, respectively).

4) Modification of the AFM tip

Figure 5 shows a schematic of the procedure employed to attach a mineral particle to the commercial AFM cantilever. First, the glue and then a single particle are picked up by the AFM tip from a standard microscope slide. Then, the glue is hardened under UV radiation by 1 h. This is a modified version of the dual wire method proposed by Y. Gan [6]. Scanning electron microscopy (SEM) and energy dispersion spectroscopy (EDS) were used to verify the quality of each modified AFM tip (Fig. 5, bottom).

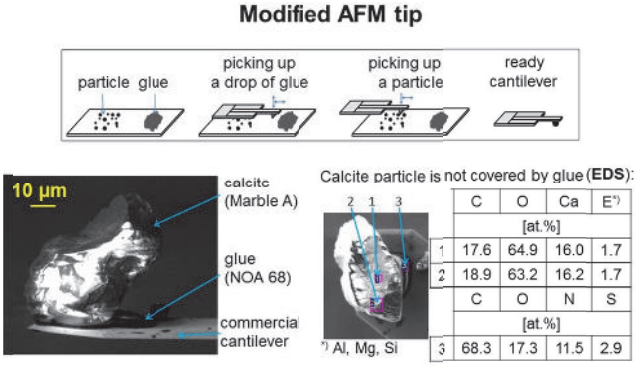

Fig. 5 *Scheme of the procedure of attaching a mineral particle to the commercial AFM cantilever (upper). A SEM image of the modified AFM tip (bottom left) together with EDS analysis which controls purity of the modified AFM tip (bottom right) (by courtesy of Dr. Kartik Pondicherry).*

An example of rubbing a calcite particle against a calcite (100) single crystal surface with a low contact force is presented in Fig. 6. The surface potential changed maximally by -4 V. Also, a decay of the introduced charge is observed.

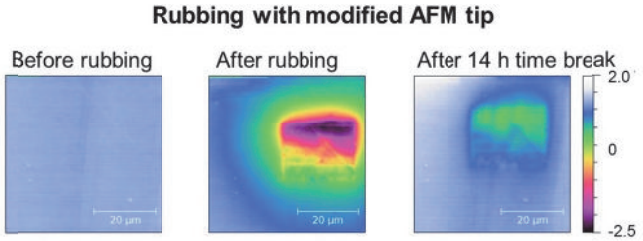

Fig. 6 *50x50 µm² KPFM images of a calcite (100) single crystal before and after rubbing with a calcite microparticle attached to the commercial AFM tip. Rubbing was performed on area of 20×20 µm² with a force of 0.01 µN.*

Cooperation:

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Dr. Kartik Pondicherry (Chair of Mechanical Engineering, Department Product Engineering, Montanuniversitaet Leoben)

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Micro four-point probe (M4PP) investigations on ZnO varistor ceramics

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Varistors are electroceramic components which show a typical current-to-voltage *(I-V)* behavior $I \propto V^{\alpha}$ with strongly increased values for α above a certain switching voltage of about 3 V. This effect is caused by so called double Schottky barriers at the grain boundaries in the polycrystalline ZnO. In previous work, Conductive Atomic Force Microscopy (C-AFM), Scanning Surface Potential Microscopy (SSPM) and Kelvin Probe Microscopy (KPFM) have been employed to study transport properties of individual grain boundaries [1] which could reveal voltage dependent current paths [2].
Here, we utilize a Micro Four-Point Probe setup (M4PP) to characterize the electrical properties of individual grain boundaries in a praseodymium doped ZnO varistor ceramic with an average grain size of 10 µm [3].
This work was performed in collaboration with EPCOS TDK, Deutschlandsberg, Austria in the framework of the FFG bridge project (#824890) "Correlation between microstructure and macroscopic electrical properties in ZnO varistors" under the coordination of Prof. Peter Supancic, Institute for Structural and Functional Ceramics, Montanuniversität Leoben.

1) M4PP set-up

M4PP overcomes several limitations of the scanning probe microscopy based approaches by separating the current and the potential measurement as is illustrated in Fig. 1. The setup consists of digital microscope and a Keithley dualsource meter. All measurements were performed with microfour-point probes from CAPRES. These probes are four gold coated, flat, 3 µm wide, and 25 µm long silicon cantilevers mounted on a single chip. Their typical spring constant is 5 N/m and their center-to-center distance is 5 µm. Thus, a minimum grain diameter of 8 µm is required for measurements as can be seen in Fig. 1 which shows an optical micrograph of the probe positions for a ZnO grain boundary measurement. The probes are positioned by the micromanipulator in a way that the grain boundary under investigation is between the two inner probes. The outer probes are placed within the same grain area as the adjacent inner probe. A voltage was applied between the outer probes (1 and 4) and the resulting current between these electrodes was recorded. In addition, the voltage drop between the inner probes (2 and 3) was measured. Due to the high conductivity of doped ZnO, the resistivity within one grain is negligible and the entire resistance is considered to originate from the grain boundaries.

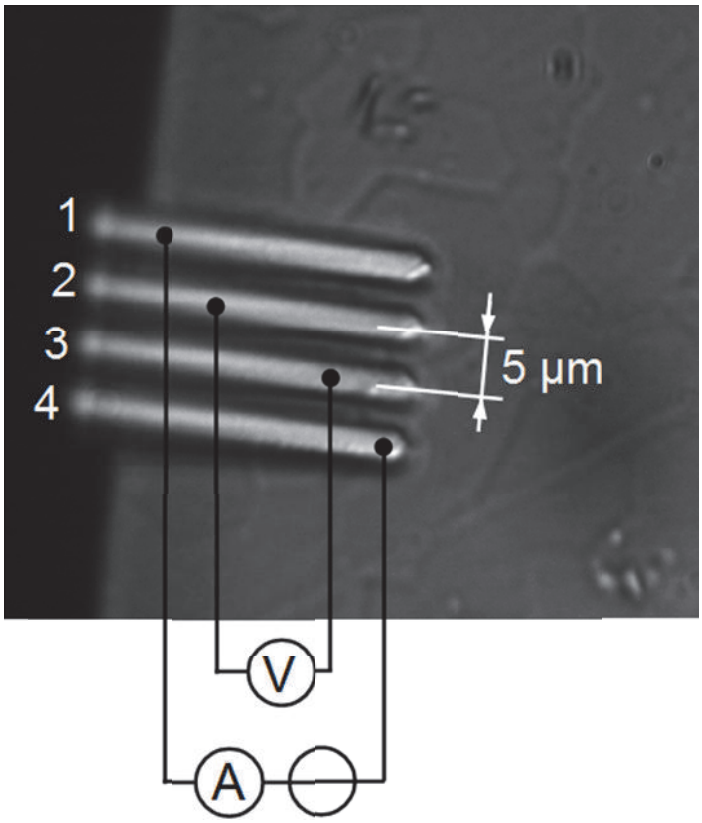

Fig. 7 Optical micrograph of a polycrystalline ZnO varistor ceramics with a scheme of the electrical setup and the M4PP probes (from [3].)

2) Results

Fig. 2 shows an I-V measurement for one exemplary grain boundary in a double logarithmic plot. For the measured curves, three different electrical regimes with different slopes (α, β and γ) can be defined. Two regimes are in the high resistive leakage region below the breakdown point with the voltage at breakdown VBD and the current IBD and a third region is above the level of Schottky barrier breakdown. Forward direction (FWD) means that a positive voltage is applied to the first probe and BWD denotes the application of a negative voltage. All measured curves exhibited a pronounced asymmetric behavior with significant differences for the values in FWD and BWD.

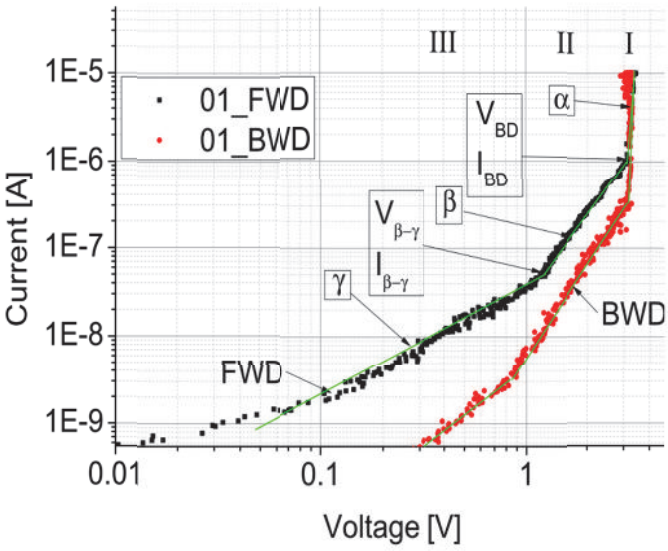

Fig. 8 M4PP measured I-V curve of one exemplary grain boundary in a multilayer ZnO varistor with the values for statistical analysis (From [3]).
The slope in region I, α, and the voltage at breakdown, V_{BD}, are the most important values to characterize the varistor behavior.
To obtain a statistical overview of these values, the data from 41 grain boundaries (82 curves in FWD and BWD) are presented in Fig. 3. For the α values, a spread from below 10 up to 150 was found. For the different grain boundaries, a spread in the breakdown voltage from 2.3 V to 3.6 V and for the breakdown current from ~ 0.05 µA to a few µA was found. The also investigated ZnO–electrode junctions showed a spread from Ohmic and symmetrical to nonlinear and asymmetric behavior.

In order to obtain frequency dependent information on the transport properties across grain boundaries, during a granted research stay at the Center of Nanophase Materials Science, Oak Ridge National Laboratory, Scanning Impedance Microscopy was employed and further on also established at the Scanning Probe microscopy Group in Leoben. The technique allows the observation of frequency dependent, non-linear transport properties in the high-resistance regions as well as measurements in the low-resistance region of the barriers.

Cooperation:

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Christoph Auer, Andreas Bürgermeister, Christian Hofmann, Monika Piber, and Manfred Schweinzger, EPCOS TDK, Deutschlandsberg, Austria
Evgheni Strelcov and Sergei Kalinin, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oakridge, TN, USA.

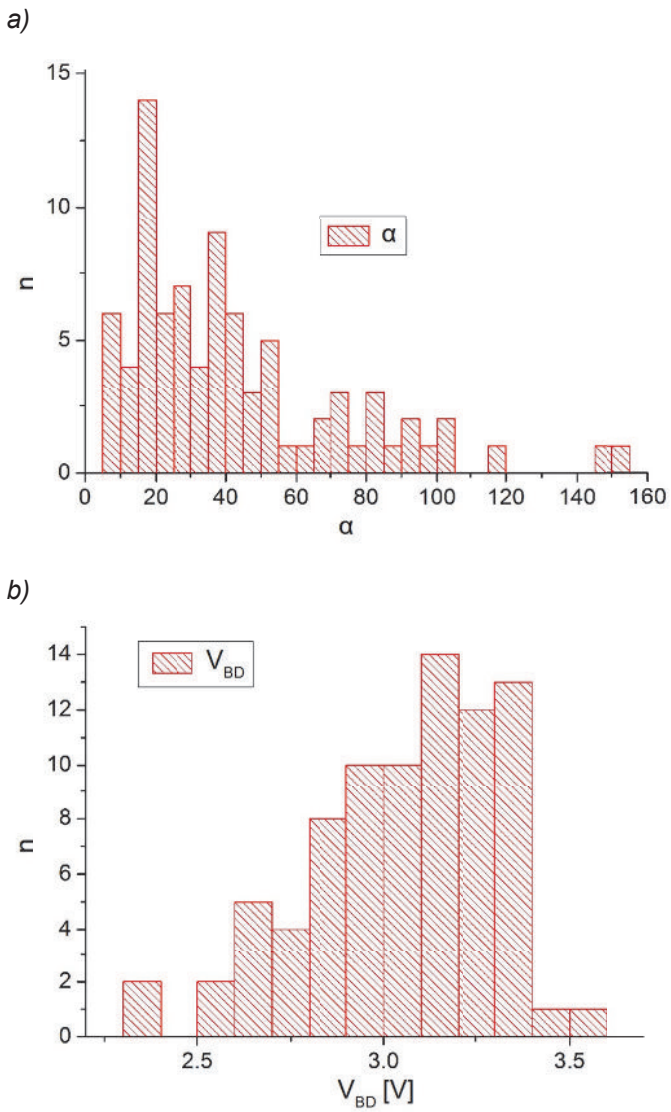

***Fig. 3**: Histograms of the most crucial device parameters of 41 grain boundaries in a ZnO multilayer varistor with a) slope α (exponent) in region I; b) Voltage at breakdown V_{BD}. (After [3].)*

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Photoresponse of single nanorystals investigated by photo-conductrive atomic force microscopy

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To meet the demands of next generation electronic and optolectronic devices novel semiconductor materials have to be developed. Requirements like high speed, low power consumption, high integration, and low production costs have to be fulfilled. One line of approach is the use of low dimensional semiconductor nanostructures like nanodots, nanowires, and nanorods. These nanostructures can be manufactured form inorganic materials like Si, Ge, ZnO, InAs, etc. but also form organic compounds like parahexaphenyl, pentacene, C_{60}, or graphene.
For the development and integration of such nanostructures, proper nano-scale characterization methods are essential. Modern scanning probe based techniques like conductive atomic force microscopy (C-AFM), photo-conductive atomic force microscopy (PC-AFM) or Kelvin probe force microscopy (KPFM) are available for proper electrical and photoelectrical investigations of the nano-systems.

1. Self-assembled Ge nanodomes on Si(001)

Support: ÖAD Project UA 11/2009;
FWF Project # P19636-N20, NASU Project # 9/07, Ministry of Education and Science of Ukraine Project # M/34-09

Ge/Si(001) is an intensively studied model system for lattice mismatch driven self-assembly. Deposition of Ge on a crystalline silicon substrate yields a spontaneous formation of 3D nano-crystals with interesting charge carrier properties [1].
Here, we investigate such electrical and photovoltaic properties of self-assembled Ge nanodomes (ND) on Si(001). A high resolution AFM topography image of a typical ND presented in Fig. 1 reveals the existence of well oriented facets. Based on a facet angle analysis {113} and {15 3 23} facets could be unambiguously attributed. Further, indications of {105} and {001} facets are found.
In Fig. 2, a photocurrent map (0V bias, illumination with 860 nm light) together with the simultaneous measured topography of several NDs is presented. Clearly a correlation of the photocurrent and the facet structure can be made. Photocurrent maxima appear at the transition between the {113} and {15 3 23 facets} whereas the photocurrent is significantly smaller at the {113} facets.

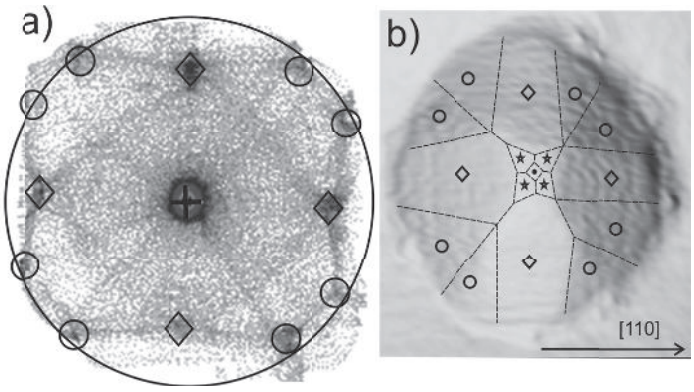

Fig. 1 *(a) Frequency of occurrence and orientation of planes with their angular orientation with respect to the surface normal) calculated from a 1.5 × 1.5 µm² tapping mode AFM image. The facets are indicated by open diamonds ({113}) and circles ({15 3 23}). (b) Intermittent contact mode AFM image of a single Ge ND on Si(001) in 3D presentation with assignment of the facets (★{105}, •{001}, ♦{113}, ◦{15 3 23}).(from [2])*

A further characterization of the photoresponse of the NDs was performed by measuring current-to-voltage (IV) curves on top of individual NDs of different diameter.
In Fig. 2, typical IV curves in dark and under illumination of a ND with a diameter of 103 nm are presented. The inset in Fig. 2 clearly reveals the short circuit current I_{SC} and the open circuit voltage V_{OC} generated under illumination.

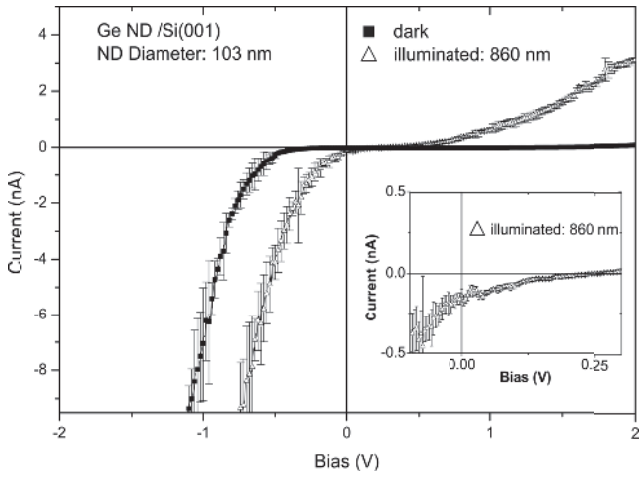

Fig. 2 Current-to-voltage characteristics measured on top of a single Ge nanodome with a diameter of about 100 nm in the dark (black squares) and under illumination (white triangles). The inset presents the low positive bias region under illumination with enlarged scale. (from [2])

2 Photresponse from single ZnO nanorods

C-AFM and PC-AFM were applied for the characterization of individual as grown n-type ZnO nanorods (NR) [3]. Due to its wide band gap of 3.37 eV, ZnO has potential applications in ultraviolet optoelectronic devices like solar cells, lasers, LEDs, photodetectors, etc. Additionally, gas adsorption significantly alters the electrical properties of the

surface near region making nanosize crystals with high surface to volume ratio ideal candidates for gas sensing applications. ZnO also features the so called persistent photoconductivity (PPC) which means a very slow recovery to the dark level conductivity after illumination. In Fig. 3, the transient photoresponse of an individual upright standing NR upon cycling illumination is presented.

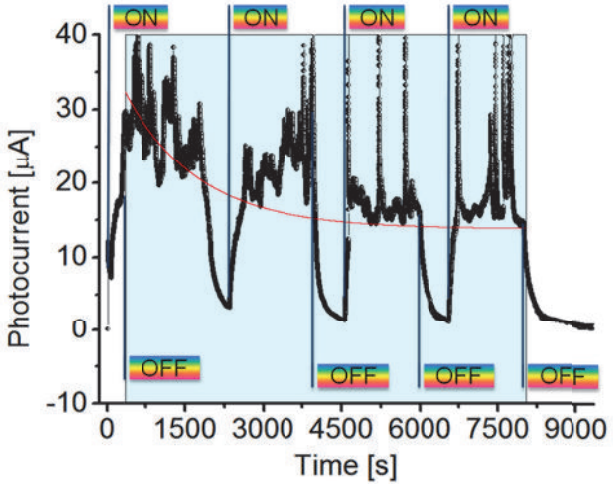

Fig. 3 *Photocurrent rise and decay due to several cycles of illumination. Sample bias -10 V, the source of illumination is a 150 W Xe lamp (white light). The flags mark the light-on and off switching.(from [3])*

The return to the dark current value takes several 100 s and can be well fitted by an exponential decay with a time constant of τ=140±20 s. The PPC in ZnO is often described as a surface effect associated with an electron-hole pair generation and subsequent recombination of the hole h^+ with adsorbed O_2^- species.[4] This model also implies that PPC in ZnO is limited to the fundamental adsorption range (super band gap illumination). However, the photoconductivity spectral response measured on the same rod (not shown) reveals a photocurrent onset already at photon energies of 3.1 eV which is 0.27 eV smaller than the band gap. The slow kinetics together with the sub band gap response is in contradiction to the generation of electron hole pairs and subsequent oxygen desorption. In fact our findings supports a different model that involves oxygen defect states (defect localized states, DLS and perturbed host states, PHS) in the band gap close to the valence band edge as proposed by Lany and Zunger [5]. The process is schemed in Fig 4.

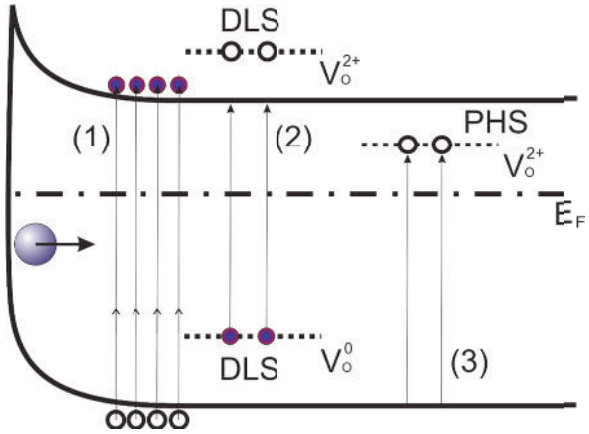

Fig. 4 Schematic energy-level diagram of ZnO taking into account the existence of theoretically predicted [5] a- and b-type configurations of oxygen vacancies. The processes of electronhole pair generation via band-to-band absorption, charge carrier photo-excitation from defect localized state (DLS) and to perturbed host state (PHS) of oxygen vacancy are marked as (1), (2), and (3), respectively.(adopted from [5])

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Photonics and Nanoelectronics

Photonics for Optoelectronics and Mining Applications

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1) Simulation of Hybrid Metal Dielectric Couplers for Optoelectronics

Integrated Photonics makes it possible to join infrared optical (e.g. λ = 1.55µm) signals transmitted by fibers with detectors and sources in (predominantly silicon based) integrated circuits. To optimize the coupling between these elements intermediate structures are needed. Wan et al. [1] proposed a hybrid coupler composed of a dielectric slab waveguide and a thin metallic strip (cross section shown in Fig.1):

Proposed coupler:

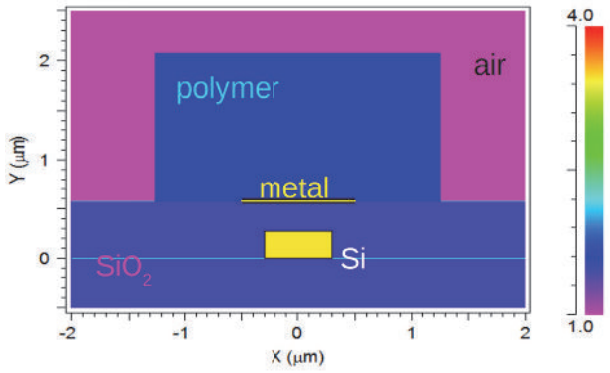

Fig1.: Cross section of hybrid coupler for infrared waves from a Si dielectric slab to the metal strip above. Color scale indicates real part of the refractive index

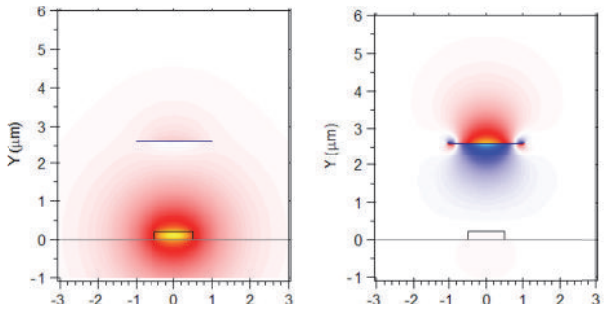

Fig. 2 : *Cross section of magnetic field distribution (H_z) of the individual Si dielectric slab (left) and metal wave guide modes (right). The colors red (yellow for strong fields) and blue indicate opposite polarities of the field.*

We performed finite element calculations and obtained the modes corresponding to the dielectric slab wave guide (Fig.2 left diagram) and metal wave guide (right) are not coupled. Putting the wave guides in close proximity these modes couple to form hybrid modes ψ_A and ψ_B (see Fig.3). To optimize this coupling, the geometry of the waveguide is chosen so that the individual guides have the same phase velocity. The coupling introduces a split in the phase velocity of the two hybrid modes. Due to the difference in phase velocity, causing a relative phase shift between the modes, a superposition of both modes will oscillate along the guides from being concentrated at the dielectric wave guide (Fig.4 left) to being concentrated at the metallic guide (Fig. 4 right) and back again. In this way letting the two guides overlap for half the beat distance allows a transfer of the wave from the dielectric guide to the metal strip as shown for a pulse in Fig. 5.

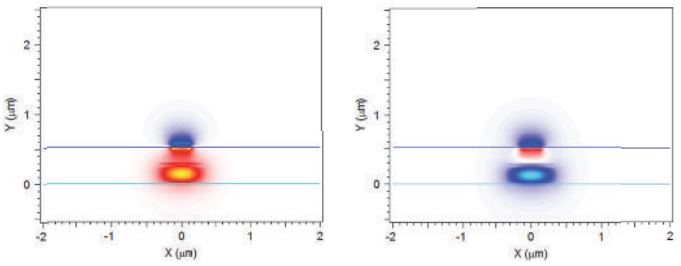

Fig. 3: *Field distributions of the coupled modes ψ_A (left) and ψ_B (right) of the hybrid metal dielectric coupler.*

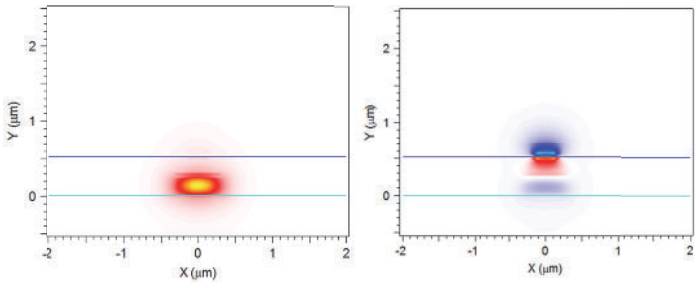

Fig. 4: *Field distributions of odd ($\psi_A - \psi_B$.) and even ($\psi_A + \psi_B$) superpositions of the coupled modes of the hybrid metal dielectric coupler.*

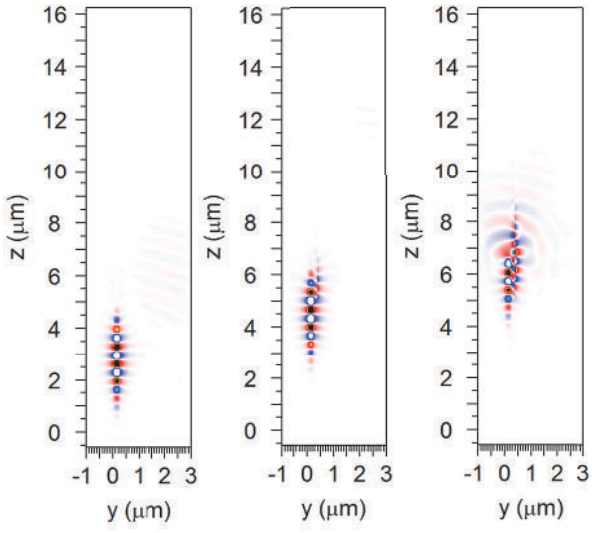

Fig. 5: *Pulse initially induced in the dielectric waveguide (left diagram) coupling to the metallic guide shown for subsequent times.*

Cooperation: W. Jantsch, T. Fromherz, M. Humer (Institute of Semiconductor and Solid State Physics, Johannes Kepler University, Linz).
O. Glushko (Erich-Schmid-Institute of Materials Science ESI, ÖAW, Leoben)

2) Microwave absorption in heterogeneous solids – simulation and experiment

Motivation:
The process of fragmenting rocks for mining, building of tunnels, or the extraction of valuable minerals is very energy intensive. E.g., in the USA it is responsible for 29% of the energy consumption in mining. It is responsible for up to 2% of the total energy consumption. Most of this energy is lost - only 1% is used for the formation of new surfaces. It is therefore of great interest to weaken the cohesive structure of the rock. One way to achieve this is the generation of internal stresses by the internal creation heat using microwaves. The aim of this work is to study how the microwaves propagate in the rock. This yields the distribution of the electromagnetic field and enabling to determine the absorbed power within the rock. The absorbed power is used to model the temperature increase which furthermore induces stress by temperature gradients and by differences of the coefficients of thermal expansion in the different materials constituting the rocks.

Model:
To simulate the electromagnetic properties of rocks a two component model is used [3]: One component is the matrix with dielectric constant κ_m surrounding inclusions (with dielectric constant κ_d). The model is two-dimensional, i.e., the dielectric constant varies only in two dimensions (chosen to be the x- and z-direction) and is constant in the third (y) direction. In the model the inclusions are cylindrical (with circular cross section) (see Fig. 6).
To determine the effect of the inhomogeneity on the propagation in the two-component material is compared with the propagation in a homogeneous material with an equivalent effective dielectric constant $\kappa_{eff.}$ It obeys the Bruggeman equation[4]:

$$f\frac{\kappa_d-\kappa_{eff}}{\kappa_d+(d-1)\kappa_{eff}}+(1-f)\frac{\kappa_m-\kappa_{eff}}{\kappa_m+(d-1)\kappa_{eff}}=0$$

f is the filling factor – the fraction of the volume occupied by the inclusions. d is the dimensionality of the system. This equation can be used to determine κ_{eff}:

$$\kappa_{eff}=\hat{\kappa}+\sqrt{\hat{\kappa}^2+8\kappa_d\kappa_m} \text{ with}$$

$$\hat{\kappa}=(1-df)(\kappa_d-\kappa_m)+(2-d)\kappa_m .$$

Conversely, κ_d can be adjusted for a chosen κ_{eff}:

$$\kappa_d=\frac{((d-1)-df)\kappa_m-(d-1)\kappa_{eff}}{-\kappa_m+(1-df)\kappa_{eff}}\kappa_{eff}$$

Assuming a background dielectric constant of κ_m = 7.1, a $\kappa_{eff.}$ = 7.4 + 0.88i is achieved with inclusions with $\kappa_{d.}$ = 7.69+2.787i.
The source is modeled by a Gaussian beam of 8.6 cm width emitting microwaves with a frequency of 2.45 GHz.

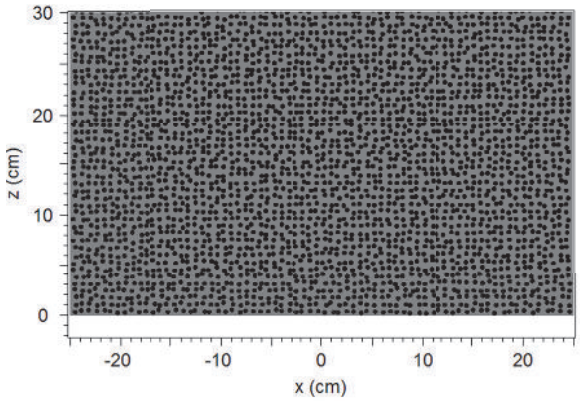

Fig. 6: *Two-dimensional model of the rock consisting of two materials: The matrix (shown light grey) and circular inclusions (dark grey).*

Method:
To calculate the propagation of electromagnetic wave the finite difference time domain (FDTD) method [5,6] is employed. This method discretizes Maxwell's equations. It determines the electrical and magnetic fields at time t+Δt from the fields at the previous time t allowing to directly observe the propagation of the fields. The FDTD calculations are performed using the FDTD programs FullWAVE by RSoft[7] and meep (developed at the MIT)[8].
3D calculations require, due to the additional dimension, vastly larger RAM storage. First simulations were performed on a PC with 16 GByte RAM. A cluster system at the Montanuniversitaet allows to perform calculations on many computers (so-called nodes) in parallel. Each node has 128 GByte RAM.
To determine the distribution of the absorbed energy as input for the determination of the temperature rise the average absorbed power density $\langle P_{abs}\rangle$ has to be determined from the electric field **E** by the relation $P_{abs}=\omega \mathrm{Im}\kappa|\vec{E}|^2$. In this two-dimensional model E is oriented along the y-direction. It is therefore important to examine E_y^2.
When the microwave radiation has fully propagated into the material (after about t=24T, T is the period of the microwave) and the $|\mathbf{E}|^2$ pattern, averaged over a period, has stabilized, it is sufficient to integrate over one period. Furthermore, for a harmonic wave, it is only necessary to determine $|E_y|^2$ at two times t and t+T/4.
These results are then used to determine the change in temperature due to the absorbed power and subsequently the development of internal stresses using the ABAQUS software [9]. The calculations were performed at the Institute of Mechanics.

Results:

The results of the time averaged E_y^2 distribution are shown in Fig.7. This distribution allows to determine how far the microwaves propagate into the material. To show the effect particular to the heterogeneity of the material, in Fig. 8 the difference to the equivalent homogeneous case is displayed. There is increased intensity to the sides of the beam due to sideways scattering and a reduction of the intensity further into the material.

From the E_y^2 distribution the absorbed power density P_{abs} is determined (see Fig. 9)

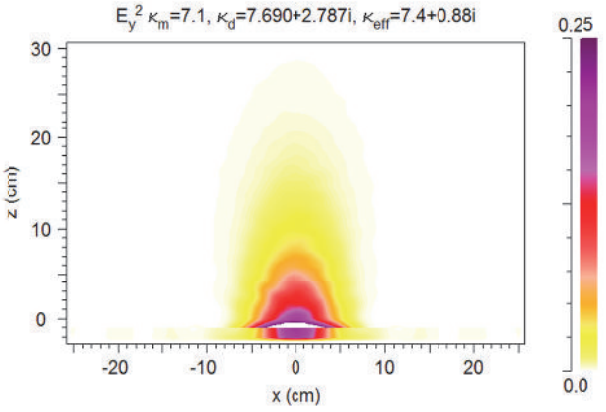

Fig. 7: *Distribution of E_y^2 demonstrating how far the microwave beam propagates into an inhomogeneous rock. (κ_m=7.1, κ_d=7.69+2.787i).*

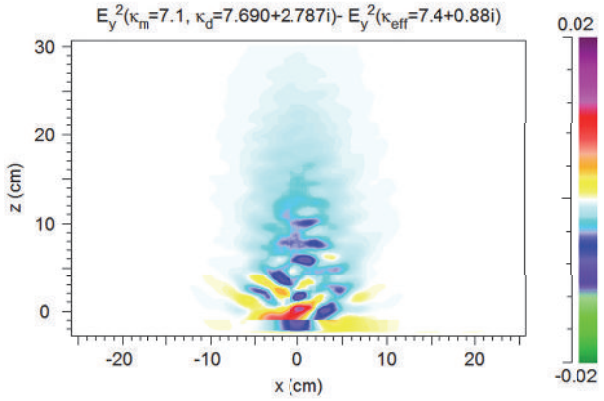

Fig. 8: *Difference of E_y^2 between inhomogeneous (κ_m=7.1,κ_d=7.69+2.787i) and homogeneous (κ=κ_{eff}= 7.4+0.88i) material.*

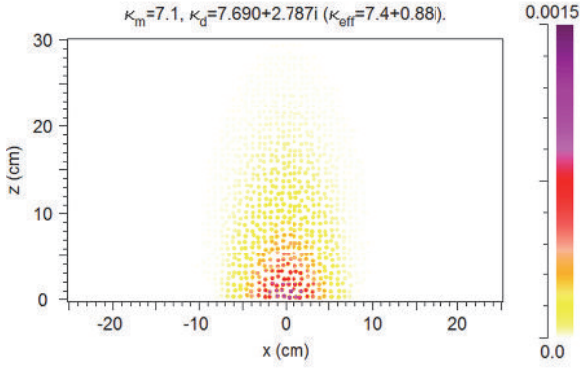

Fig. 9: *Absorbed power density for the inhomogeneous material.*

To investigate the origin of fluctuations due to the inhomogeneity of the material, the distribution ΔE_y^2 of the difference between the inhomogeneous and the homogeneous material is compared with the positions of the inclusions (see Fig.10). Because the wavelength of the microwaves is much larger than the size of the inclusions the smoothed density of the inclusions may also be the target of the comparison (see Fig. 11).

Neither the arrangement of the disks nor their density shows a correlation with the details of the pattern of ΔE_y^2.

The possible origin of the ΔE_y^2 fluctuations can be seen more clearly for a case with lossless inclusions with stronger deviation from the matrix (Fig. 12). Due to absence of absorption the waves propagate deeper into the material. This material shows the fluctuations more distinctly with a stripe-like nature. The distance between the stripes is about half the effective wavelength $\lambda_{eff} = \frac{c}{f}\sqrt{\kappa_{eff}}$. Such a pattern would arise by interference between the incident wave and the waves coherently backscattered at the randomly distributed inclusions. This process is also responsible for the Anderson localisation.

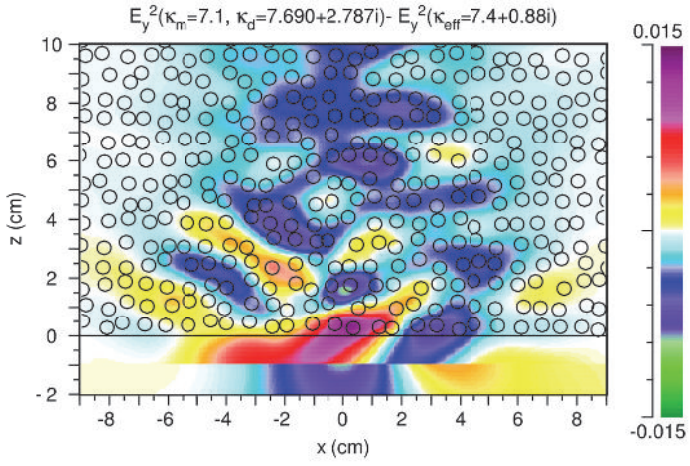

Fig. 10: *Comparison of the E_y^2 distribution with the positions of the inclusions.*

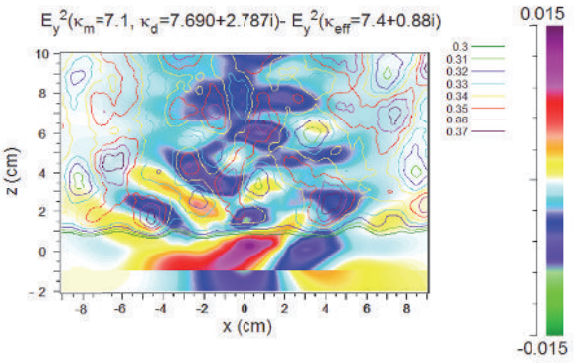

Fig. 11: *Comparison of the E_y^2 distribution with the smoothed inclusion density fluctuating around the filling factor f= 0.34.*

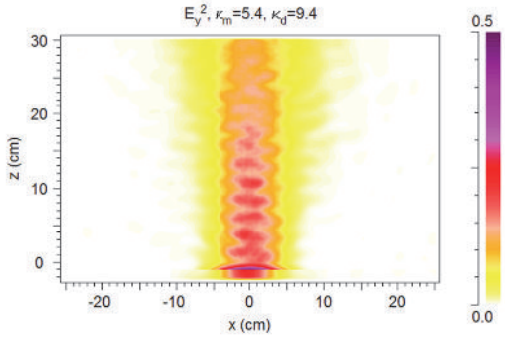

Fig 12: *Distribution of E_y^2 for the lossless case κ_m=5.4, κ_d=9.4 showing a stripe-like pattern.*

Only for strong differences in the dielectric properties the deviations from the Gaussian broadening are significant.
From the E_y^2 distribution of the absorbed power density P_{abs} (shown in Fig. 9)in the beam the time dependence of the temperature and the stresses are 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.

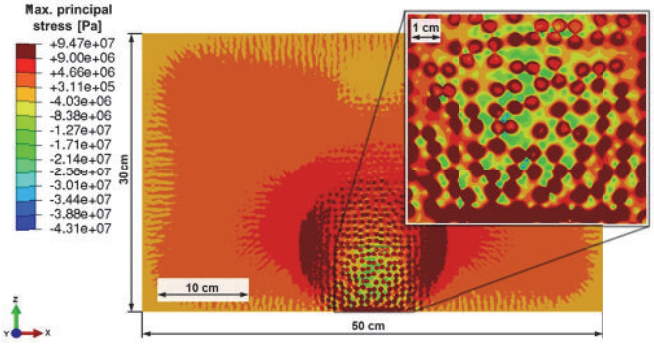

Fig. 13: *Maximum principal stresses in the model rock after 15 s of microwave irradiation (2.45 GHz, 17.5 kW) calculated from the distribution of the absorbed microwave power and the resulting temperature distribution. Dark red indicates values larger than 9 MPa.*

3D simulations:

The calculations were extended to the fully three-dimensional case. In this case the inclusions are modeled by randomly positioned spheres with dielectric constant κ_d in a matrix with dielectric constant κ_m.

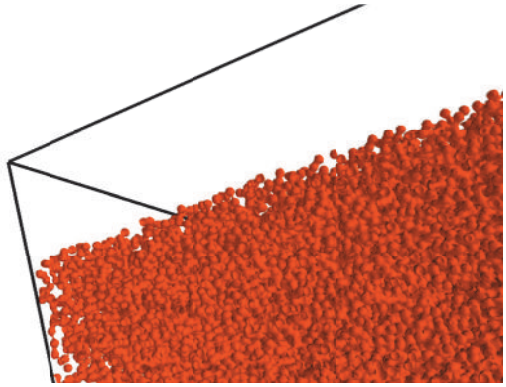

Fig. 14: *Spherical inclusions (red) randomly filling the matrix (not shown for clarity).*

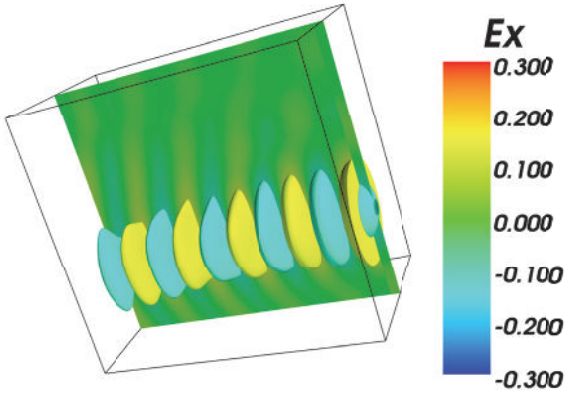

Fig. 15: *Snapshot of the propagation of a Gaussian beam in the modeled material. To reduce the memory requirements the simulation domain is truncated in lower part.*

Experiment

In order to validate the numerical models qualitatively experiments on various kinds of hard rock were performed with high-power microwaves at 2.45 GHz. A block of rock (50x50x30 cm^3, 30 cm in the direction of microwave propagation) was irradiated using an open-ended rectangular waveguide as the applicator. The block of rock was positioned on an x-y table encapsulated in a cage preventing stray radiation reaching the surrounding and the operating personnel. The opening of the applicator was 4.3 x 8.6 cm^2. Due to the field distribution in the waveguide and a few centimeters distance between waveguide and rock the area of the irradiated spot on the rock is rounded. The region of high intensity is indicated by a circle with 5 cm diameter in Fig.16 [10,11]. The two examples show spallation of basalt and cracking of gabbro. This indicates that both types of damage can occur but that the details depend on the type of rock, in particular on its thermal and mechanical properties.

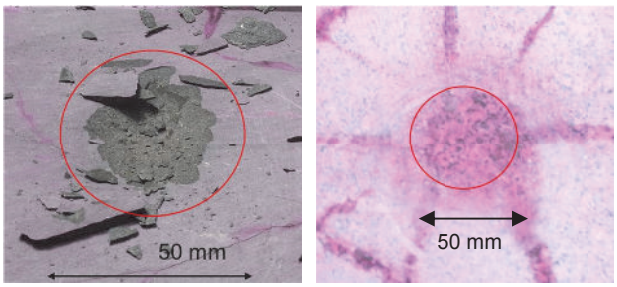

Fig. 16: *Damage of basalt (left) and gabbro (right) after irradiation with 2.45 GHz microwaves at 17.5 kW for 15 s and 72 s, respectively [10,11]. The circle indicates the irradiated area.*

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M. Toifl, T. Antretter, Institute of Mechanics, Montanuniversitaet Leoben.

Funding:

(FFG project number 820125/18797; FWF project TRP 284-N30).

3) Magnetic-Field Tuning of Photonic Crystals

Tuning the flow of light by external fields is a challenging task for scientific studies and optical applications. It is important in many applications such as switches, modulators, and slow-wave structures. Here, numerical and experimental results are presented which demonstrate that this effectively can be achieved by external magnetic fields in one-dimensional photonic crystals (PhC) made from semiconducting material. The advantage of using semiconducting material is the magnetic-field dependent dielectric function of the free charge carriers particularly where the magnetic field causes large and strongly varying contributions – near the plasma frequency and the cyclotron resonance frequency. The results of simulations on the basis of a multiple scattering method at infrared and microwave frequencies and of experiments on Indium Antimonide in the latter frequency regime confirm the tunability up to the extreme case from full transparency to opaqueness and vice versa.

The calculations of the transmittance, reflectance, and absorbance of a one-dimensional PhC containing plane parallel slabs of a material with free carriers in a magnetic field were performed by applying the multiple scattering method and using a modified version of the program MULTEM2 [12]. The propagation of the radiation was parallel to the external magnetic B field and perpendicular to the plane of the slabs. A result for cyclotron resonance active (CRA) circular polarization is shown in Fig. 17 [13].

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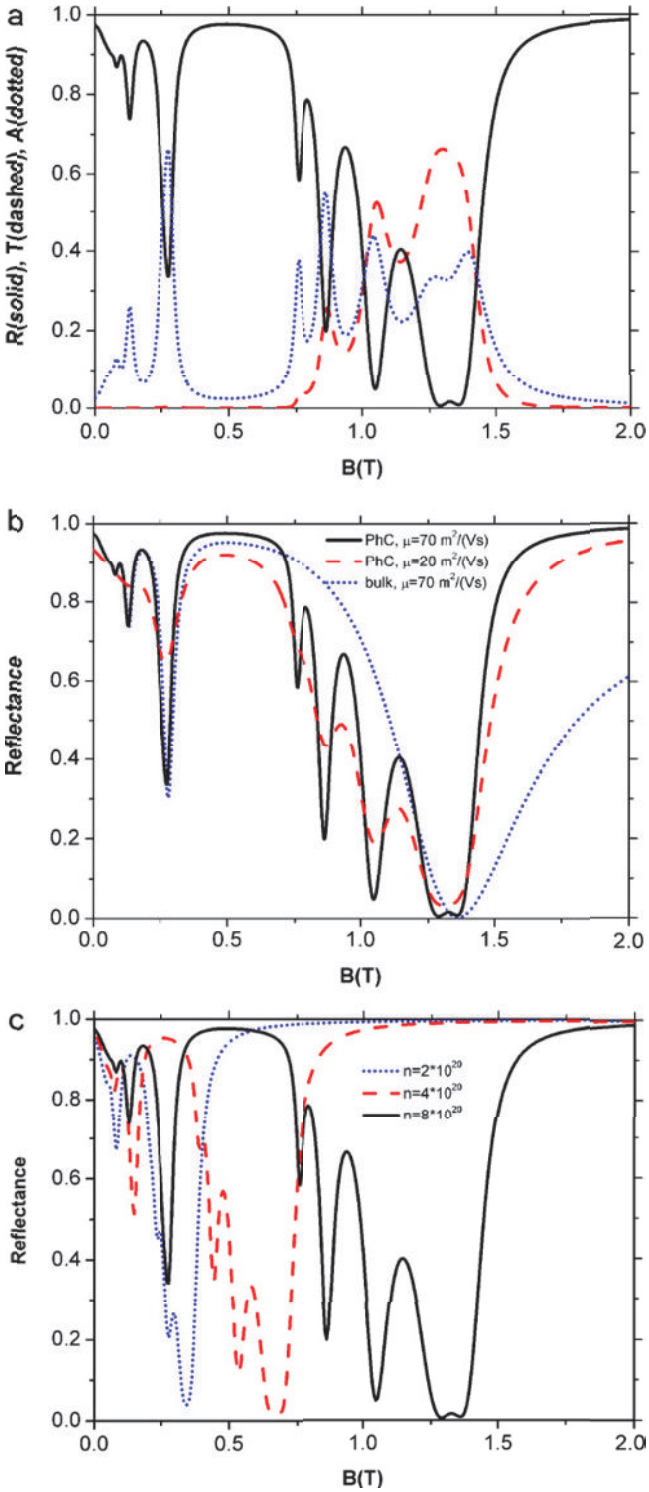

Fig. 17. *(a) Calculated transmittance T, reflectance R and absorbance A for the InSb/air PhC at f = 38 GHz, i.e. below the plasma frequency (f_p = 523 GHz). n = 8 x10^{20} m^3, m = 70 m^2/Vs. (b) Dependence of the reflection of the PhC on mobility and comparison with bulk InSb (thickness 500 mm), n = 8 x 10^{20} m^3. (c) Dependence on carrier concentration, m = 70 m^2/Vs. All diagrams are for CRA polarization.*

Simulation Electric Transport

Modelling of quantum electron transport in high magnetic fields

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The actual research activities concerning modelling of quantum electron transport in high magnetic fields are a result of our long term research activities that started with epitaxial growth and experimental magneto transport investigations of 3D and quasi 2D electron systems (wide quantum wells and doping super lattices) based on narrow gap semiconductors. A major goal from the very beginning was the investigation of the magnetic field induced metal insulator transition and Wigner condensation of electrons, which is also an important ingredient of the quantum Hall effect in 2D electronic systems. In this context the physics of the quantum Hall regime was a continuous driving force while shifting the research activities more and more from experiments to theory and simulation. The unique electronic regime of wide quantum wells, which can be understood as an intermediate regime between 2D and 3D, demanded novel theoretical approaches to electron transport since neither 3D physics nor well defined 2D physics could be applied to our self-grown wide quantum wells.

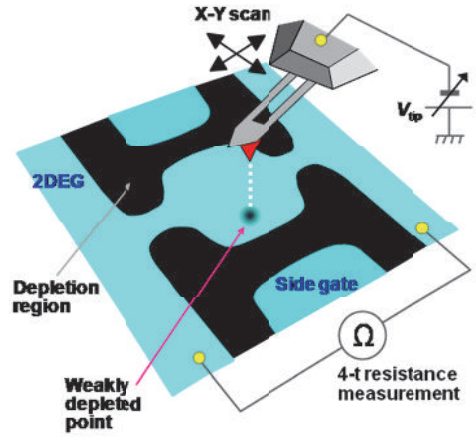
Besides the quantum Hall effect, also magneto resistance fluctuations, magneto conductance fluctuations and so called edge channel transport are important indications of the quantum nature of magneto transport. A very fundamental challenge of any theoretical approach to these effects is the fact, that the underlying electron systems consist of a many particle quantum state, while the transport for investigating these electron systems is driven by non- equilibrium, that is introduced by the contacts. Since stationary quantum states do not directly provide transport, different methods have been developed by different schools in order to overcome this counterintuitive requirement.

We have been able to contribute another new approach to non-equilibrium transport that provides also the possibility to combine it with nearly every model for the steady state of the underlying electron systems. A detailed presentation and discussion of our model in contrast to other so far existing models can be found in [1]. We started a cooperation with the group of R. Römer at Warwick University, who are experts for the calculation of stationary many particle quantum states and made plans for joining their Hartree-Fock (HF) model and our non-equilibrium network model (NNM) for transport. The idea to join these models has already been announced in an early common paper [2]. However, no clear concept had been at hand for this purpose at that time, which took several more years. Meanwhile the non-equilibrium network model has been successfully used on the basis of a semi classical approach to the microscopic nature of the electron system, as can be seen in Ref. 3

Quite a number of extensions and modifications had to be made for achieving the present status of our simulation model. That was necessary not only for handling the data transfer between the HF model and the NNM, but also in order to account for the physical boundary conditions as given under real experimental conditions. By extensive testing in the last two years it turned out that mainly two adaptations had to be made for the HF model: (i) Introducing a smooth Fermi edge in order to account for finite temperatures for the occupation of the quantum states; (ii) Introducing a predefined Fermi energy into the HF procedure instead of fixing the number of electrons in the electronic system, as done before. This is necessary because in real systems there always exists a 2D electron reservoir, in which the investigated structure is embedded. Such a reservoir pins the magnetic field dependent Fermi energy and leads to the effect that electrons will move in and out of the device under investigation while changing e.g. the magnetic field. Consequently also a module had to be added to the HF model, which calculates the 2D Fermi level as a function of magnetic field at given 2D carrier density for the host electron system. These improvements have finally led to more realistic results, but also improved the convergence behaviour of the self-consisted overall procedure.

Simulation of scanning gate microscopy (SGM): One major goal at present is the application of our model to SGM, which has the potential of non-invasive probing of quantum states that could become interesting in context with quantum computing. In this context also SGM combines the counterintuitive requirements of investigating stationary quantum states by using non-equilibrium electron transport. In the following we show briefly some recent preliminary results that demonstrate the application of SGM for real space imaging of condensed many particle quantum states.

In Fig.2 on the left it can be seen, that the response pattern of the total sample current reflects the geometry for the case of a condensed quantum state (Wigner crystal) shown on the right. The non-locality of the quantum state is evident from the fact, that the contrast does not depend on the distance of the tip from the QPC, where the tip hits the quantum state. The calculations have been made according to the material parameters of a GaAs System.



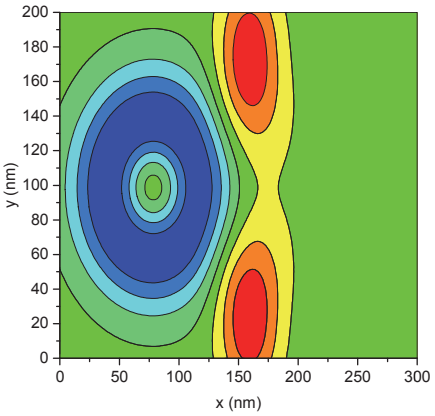
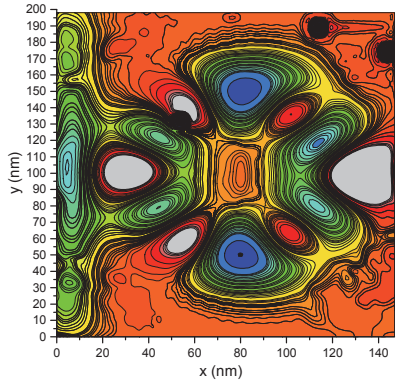


FIG.1. Left: Scheme of SGM, where a biased tip scans close to the surface and affects the buried electron system. The conductive response of the whole device is recorded as a function of tip position. **Right:** bare electrostatic potential of the simulated model system that consists of a ring shaped quantum dot nearby a quantum point contact. This structure has to be inserted between the electrodes on the left. Red means high and blue low potential for electrons that consequently will collect in the (blue) ring.



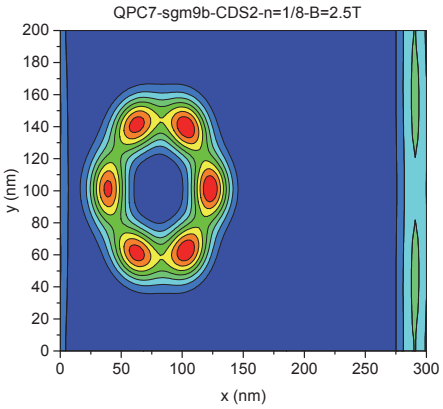


Fig.2 Left: Simulated conductive response (in arbitrary units) as a function of tip position (5mV tip potential) for the two-dimensional potential on the right of Fig. 1 that contains 8 electrons (note the different scale of the x-axis). **Right:** charge density of the condensed 8-electron many particle quantum state in the ring, that is obtained by the Hartree Fock model for the above ring potential.

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Epilogue: Future Trends in Micro- and Nanoelectronics

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The information technology industry contributes world-wide to a large extent to the gross national product and drives the economic growth of many countries, in the USA e.g. 25% and 50% respectively. The basis is semiconductor physics and semiconductor technology developed mainly during the past 70 years with the fundamental effects discovered up to a century earlier. In cooperation with with B. Kramer, University of Hamburg a review "Future Trends in Semiconductor Technology and Computer Assisted Modelling of Solids" was compiled (invited talk at Metallkundekolloquium 2014, Lech). Here, the expected trends for microelectronics are briefly described.

After the invention of the semiconductor based transistor in 1947 and the introduction of planar integrated circuits (IC) around 1960, the development of microelectronics followed Moore's law since the late 1960s. Moore's law means a doubling of the transistor count on a chip every 18 – 24 months. This was accompanied by a reduction of typical dimensions like the gate length in a MOSFET (metal oxide field effect transistor) from 10 µm to 22 nm (the "22 nm node") during the past 45 years resulting in more than 1 billion transistors on a chip. Already since the end of the 1980s microelectronics is nanoelectronics. The almost exclusively used electronic device and material were the MOSFET and silicon, respectively. Essential milestones allowing to follow Moore's law were the introductions of the planar IC, the CMOS technique (~1990) and the FinFET (2011). The planar technique enabled two-dimensional integration of electronic circuits. CMOS drastically reduced the power consumption. The FinFET concept is a step in the third dimension. With the gate on three sides of the current carrying "fin" it allows much better control of the current through the device.

These technological achievements were accompanied by achievements in theoretical solid state physics. Early attempts of computing electronic properties of semiconductors including the band structure were reviewed by William Shockley – one of the inventors of the transistor - in 1950. Since the 1960s single-electron approximations, e.g. pseudo-potential theory, were used. The actual many-electron system with about 10^{23} electrons in one cm^3 of a semiconductor is unsolvable even on the largest present-day computers. Important achievements within the recent decades in the direction of "ab-initio" theories included the Born-Oppenheimer approximation, the Hartree-Fock theory, and the density-functional theory (DFT). In DFT the ground state is calculated in single-electron approximation; the exchange interaction of the many-electron system is represented by the density or the gradient of the density. This resulted e.g. in values of the fundamental energy gaps of many semiconductors reproducing the trends from narrow-gap to wide-gap materials very well, however with the absolute values deviating from the experimental ones, e.g. by a factor of about 2 for silicon. Using many-electron methods for the excited states. i.e. many-valley Green's functions and dynamically screened Coulomb interaction, the deviation was essentially removed. These methods will be a main theoretical tool for predicting electronic properties of novel electronic materials. For instance they allow to discover whether a solid has a non-zero fundamental energy gap which is essential for electronic applications. Recently also band structures of unconventional, in many cases two-dimensional semiconductors were calculated. Several are candidates for a replacement of silicon in future micro- and optoelectronics: graphene, graphane, silicene, transition metal chalcogenides like MoS_2, just to name a few. Regarding the replacement of silicon, history tells that such a drastic step requires decades. One has to keep in mind that a new technology will have to compete with the extremely well established silicon technology producing ICs at the cost of approximately 10 US$ for 1 billion transistors on a chip. What does this mean for the development of microelectronics within the next decade?

The FinFET, also called TriGateTransistor (INTEL), will be further improved allowing to reach the 14, 10 and 7 nm node until 2024 (International Technology Roadmap for Semiconductors ITRS). It is assumed that for achieving this goal silicon will be at least partly substituted by germanium in order to reach higher electron mobility. Possibilities for realizing the 3 nm node in the 2030s are manifold. Most promising device concepts are: Si/Ge transistor with gate all around a Si/Ge wire (improved electrostatics); FinFET with Ge and III-V semiconductors as the fin material (improved electron mobility); tunneling FET with vertical semiconductor wire (improved subthreshold performance). Moore's law is expected to hold at least down to the 5 nm node – even though with some delay.

Cooperation: B. Kramer, I. Institut für Theoretische Physik, Universität Hamburg.

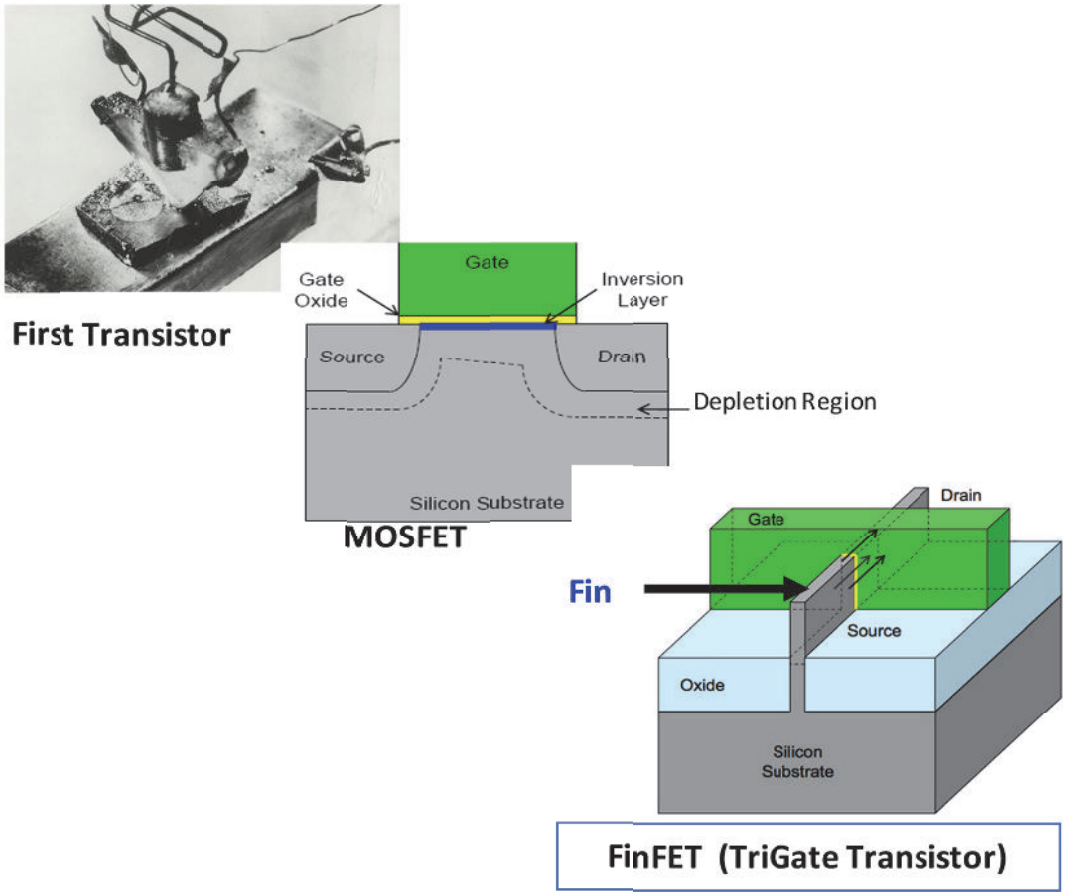

Fig. 1 The transistor pathway from 1947 to 2013

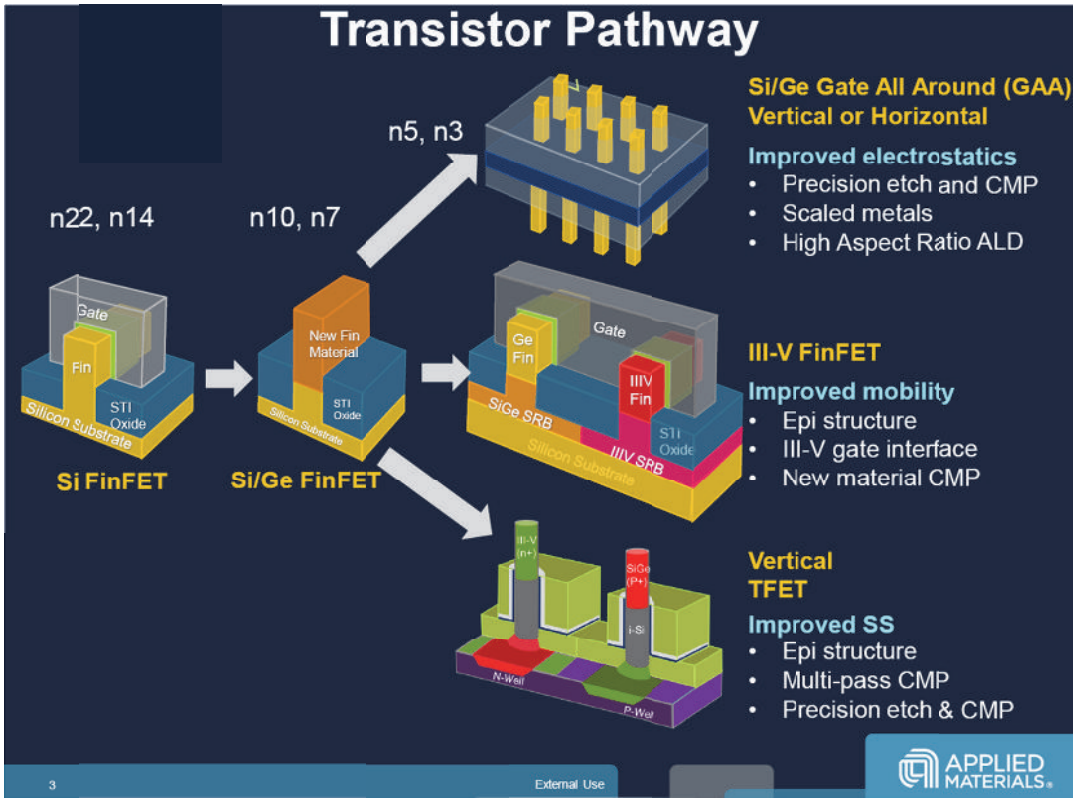

Fig. 2 *Concepts for the future transistor pathway.*

4. Publication List

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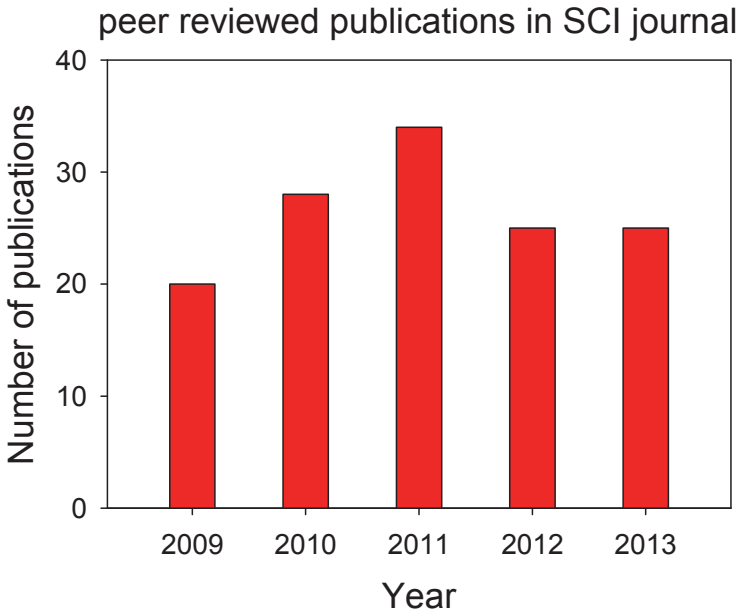
1. Lackner, J. M.; Waldhauser, W.; Schmied, F.; Teichert, C.; Keckes, J.; Kreith, J, *Biomimetik design for cell-contacting surfaces-The topographical influences on cell-biomaterial interaction and plasma-based fabrication methods for self-adapted nanostructures*: Nanostructural materials for implants and cardiovascular biomedical devices ISBN 978-83-63310-00-4 (2012) 33 – 66
2. Teichert, C.; Hlawacek, G.; Winkler, A.; Puschnig, P.; Draxl, C, *Ehrlich-Schwoebel Barriers and Island Nucleation in Organic Thin-Film Growth*: Small Organic Molecules on Surfaces Fundamentals and Applications ISBN 978-3-642-33847-2 (2013) 79 – 105
3. Hlawacek, G.; Khokhar, F. S.; van Gastel, R.; Poelsema, B.; Zandvliet, H. J.; Teichert, C., *In-situ Observation of Organic Thin Film Growth on Graphene*: Small Organic Molecules on Surfaces Fundamentals and Applications ISBN 978-3-642-33847-2 (2013) 107 - 139



5. Presentations

Talks at conferences 2012

1. Brunner, R.; Meisels, R.; Aoki, N.; Ochiai, Y.; Akis, R.; Burke, A.; Ferry, D. K., Imaging of classical trajectories and quantum mechanical states in open quantum dots, 62 Annual Meeting Austrian Physical Society. Universität Graz, 20.09.2012
2. Edler, M.; Radl, S. V.; Wolfberger, A.; Kern, W.; Rath, T.; Trimmel, G.; Kratzer, M.; Pavitschitz, A.; Teichert, C.; Marchl, M.; Zojer, E.; Schwabegger, G.; Simbrunner, C.; Sitter, H., Modulation of the Performance of Organic Devices by Means of Photochemistry, EMRS 2012. Strassburg, Frankreich, 17.09.2012
3. Fritz-Popovski, G.; Van Opdenbosch, D.; Kornprobst, T.; Plank, J.; Paris, O.; Zollfrank, C., Hierarchically structured porous ceramics and composites from nanocasting of plant cell walls, SPP 1420 Young Academy & Winter School 2012. Potsdam, Germany 18.03.2012
4. Fritz-Popovski, G.; Van Opdenbosch, D.; Zollfrank, C.; Aichmayer, B.; Paris, O., The Fibrillar and Microfibrillar Structure during Biomimetic Mineralization of Wood, Bio-inspired Materials. Potsdam, Germany, 20.03.2012
5. Fritz-Popovski, G.; Van Opdenbosch, D.; Morak, R.; Zollfrank, C.; Aichmayer, B.; Paris, O., Wood Templated Inorganic Nanoporous Materials: Formation and Water Adsorption Studied by in situ SAXS Experiments, SAS 2012. Sydney, Australien, 11.11.2012
6. Ganser, C.; Schmied, F.; Fischer, W.; Hirn, U.; Schennach, R.; Teichert, C., Single fiber-fiber bond strength measurements using atomic force microscopy, 6th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2012)., University Vienna, 11.09.2012
7. Hartmann, M.; Todt, M.; Holec, D.; Mayrhofer, P. H.; Paris, O.; Fischer, F. D.; Rammerstorfer, F. G., Mechanical stability behavior of fullerenes, DPG Jahrestagung der deutschen physikalischen Gesellschaft. Berlin, Germany, 25.03.2012
8. Hartmann, M.; Todt, M.; Holec, D.; Mayrhofer, P. H.; Paris, O.; Fischer, F. D.; Rammerstorfer, F. G., Atomistic modeling of the mechanical stability behavior of carbon canostructures, ECCOMAS., University of Vienna, 10.09.2012 **(Invited)**
9. Hartmann, M.; Todt, M.; Holec, D.; Mayrhofer, P. H.; Paris, O.; Fischer, F. D.; Rammerstorfer, F. G., Mechanical properties of carbon nanostructures investigated by Monte Carlo Simulations, Annual Meeting of the Austrian Physical Society., Karl Franzens Universität Graz, 18.09.2012
10. Hartmann, M.; Todt, M.; Rammerstorfer, F. G.; Holec, D.; Mayrhofer, P. H.; Fischer, F. D.; Paris, O., Mechanical Stability Behavior of Fullerenes, World Congress on Computational Mechanics. Sao Paulo, Brasilien, 08.07.2012
11. Kratzer, M., Electrical characterization of Ge nanodomes via AFM based techniques, DPG 2012. Berlin, 26.03.2012
12. Kratzer, M.; Vasić, B.; Gajić, R.; Teichert, C., Growth of para-hexaphenyl thin films on graphene: an AFM study, ECOSS2012. Edinburgh, Scotland, 03.09.2012
13. Kratzer, M.; Prehal, C.; Rubezhanska, M.; Kondratenko, S.; Kozyrev, Y.; Teichert, C., AFM based electrical investigations on Ge nanodomes on Si(001), ÖPG 2012. Graz, 17.09.2012
14. Kuchar, F., Wie die Metalle auf die Welt kamen, ASMET Forum for Metallurgy and Materials. Leoben, 14.05.2012 **(Invited)**
15. Kuchar, F., Vom Urknall zum Kohlenstoff - Ein Entstehungsprozess mit Feinabstimmungen, 2nd Austrian Symposium on Carbon Based Coatings. Leoben, 30.05.2012 **(Invited Plenary lecture)**
16. Lechner, R. T.; Popovski, G.; Yarema, M.; Heiss, W.; Paris, O., Core/shell profile of nanocrystals determined by anomalous SAXS, 62. Jahrestagung der Österreichischen Physikalischen Gesellschaft ÖPG 2012. Graz, 18.06.2012
17. Lechner, R. T.; Popovski, G.; Yarema, M.; Heiss, W.; Armin , H.; Schülli, T.; Paris, O., Core/shell structures of PbS/CdS nanocrystals determined by ASAXS, 15th International Small-Angle Scattering Conference 2012 (SAS2012). Sydney, Australien, 18.11.2012

18. Meisels, R.; Humer, M.; Glushko, O.; Brunner, R.; Fromherz, T., Studies on the Coupling of Dielectric and Plasmonic Waveguides using FEM and FDTD Simulations, 62 Annual Meeting Austrian Physical Society. Universität Graz, 20.09.2012
19. Meisels, R., Coupling of Electromagnetic Waves to ICs – Integrated Photonics, AMS Workshop. Unterpremstätten, 19.12.2012
20. Paris, O.; Popovski, G.; Van Opdenbosch, D.; Zollfrank, C.; Schöberl, T., Lightweight nanoporous silica and alumina from wood nanocasting: synthesis, structure, and mechanical properties , MRS Spring Meeting, Symposium SS: Structure/property relationships in biological and biomimetic materials at the micro-, nano- and atomic length scales, San Francisco, CA, USA, 13.04.2012 **(Invited)**
21. Paris, O., Biological, bio-based and biomimetic materials and their relevance for biomedical applications, 5th Vienna Biomaterial Symposium, Vienna 19.11-21.11.2012. Wien, 19.11.2012 **(Invited)**
22. Paris O., On the complementarity of SAXS and SANS, Central European Infrastructure Consortium (C-ERIC) workshop, ICTP Adriatico Guesthouse, Trieste, 11.12 - 12.12.2012 **(Invited)**
23. Teichert, C., Probing self assembly by atomic force microscopy based techniques, Int. Winter School on the "Fundamentals of Organic Electronics", Planneralm, Austria, March 3-9, 2012. Planneralm, 03.03.2012 **(Invited)**
24. Teichert, C., Rasterkraftmikroskopiegestützte Charakterisierung von Halbleiternanostrukturen, 9. Werkstoffkongress "Werkstoffe, Nanotechnologie und Anwendung, Leoben, Austria, March 28-29, 2012. Leoben, 28.03.2012 **(Invited)**
25. Teichert, C., Grenzflächen pur: Experimente mit Graphen, 58th Metallkunde-Kolloquium, Lech am Arlberg, Austria, April 16-18, 2012. Lech, 16.04.2012 **(Invited)**
26. Teichert, C., Nanostructure characterization of carbon based materials from C60 films to grphite and graphene, 2nd Austrian Symposium on carbon based coatings, Leoben, Austria May 30-31, 2012. Leoben, 30.05.2012 **(Invited)**
27. Teichert, C., AFM-based elektrical charakterization of inorganic and organic semiconductor nanostructures, European Material Research Society (EMRS) Fall Meeting 2012, Warsaw, Poland, Sept 17-21, 2012 in Warsaw (Poland), 17.09.2012 **(Invited)**
28. Teichert, C., Exploring molecular diffusion processes in organic thin film growth, 6th Vacuum and Surface Sciences Conference of Asia and Australia (VASSCAA-6), Islamabad, Oct.9-13 2012. Islamabad, Pakistan, 09.10.2012 **(Invited Plenary lecture)**
29. Teichert, C., Graphene as substrate for organic thin films, 20th Jubilee Conference in Materials and Technology, Portoro`z, Slovenia 17.-19.Oct, 2012. Portoroz, Slowenien, 17.10.2012 **(Invited)**

Talks at conferences 2013

1. Ganser, C.; Hirn, U.; Schennach, R.; Teichert, C, Using AFM nanoindentation to investigate mechanical properties of cellulose fibers in controlled humidities, 63. Jahrestagung der Österreichischen Physikalischen Gesellschaft, Johannes Kepler Universität, Linz, 03.09.2013
2. Ganser, C.; Hirn, U.; Schennach, R.; Teichert, C, Pulp fiber softening investigated at varying humidity by atomic force microscopy based nanoindentation: Zukunft.Forum Papier - Die Österreichische Papierfachtagung, Graz, 15.05.2013
3. Ganser, C.; Schmied, F.; Fischer, W.; Hirn, U.; Schennach, R.; Teichert, C, Bonding mechanisms in paper studied by atomic force microscopy based methods: 10. Werkstoffkongress, Montanuniverstiaet Leoben., 06.11.2013
4. Grießer, T.; Edler, M.; Radl, S. V.; Kern, W.; Rath, T.; Trimmel, G.; Kratzer, M.; Pavitschitz, A.; Teichert, C.; Marchl, M.; Zojer, E.; Schwabegger, G.; Simbrunner, C.; Sitter, H, Photosensitive Polymers in Organic Electronics: Towards the Modulation of the Performance of Organic Devices: Austrian-Slovenian Polymer Meeting - APST 2013. Bled, Slovenien, 03.04.2013
5. Hartlieb, P.; Toifl, M.; Meisels, R.; Kuchar, F.; Antretter, T, High-Power Microwave Irradiation of Hard Rock: 56th International Scientific Session. Sofia, Bulgaria 17.10.2013
6. Hartmann, M.; Todt, M.; Holec, D, Studying the mechanical properties of carbon nanostructures via computer simulations: GAMM - Gesellschaft für Angewandte Mathematik und Mechanik. Novi Sad, Serbien, 18.03.2013 **(Invited)**

7. Hartmann, M.; Nabavi, S, The role of sacrificial bonds on the mechanical behavior of biological materials: Euromat. Sevilla, Spanien, 08.09.2013
8. Holec, D.; Hartmann, M.; Paris, O.; Mayrhofer, P. H, Surface energy of carbon fullerenes and nanotubes; A multi-method density functional theory and monte carlo study: 84th Annual Meeting of the International Association of Applied Mathematics and Mechanics. Novi Sad, Serbien, 18.03.2013 **(Invited)**
9. Kratzer, M.; Klima, S.; Vasić, B.; Gajić, R.; Matković, A.; Ralević, U.; Teichert, C, Growth of p-6P thin films on graphene studied by AFM: DPG Frühjahrstagung 2013 Sektion Kondensierte Materie. Regensburg, Germany, 10.03.2013
10. Kratzer, M, Manipulation of single layer graphene using atomic force microscopy: 4th European Nanomanioulation Workshop 2013. Krakau, Polen, 12.06.2013
11. Kratzer, M, Modification of graphene: a case study: ÖPG, Joint annual meeting of the Austrian Physical Society and the Swiss Physical Society 2013. Johannes Kepler Universität Linz, 03.09.2013 **(Invited)**
12. Kratzer, M, Graphen als transparente Elektrode für organische Halbleiterbauelemente: Forum Licht 2013. Graz University of Technology, 05.02.2013 **(Invited)**
13. Kratzer, M.; Klima, S.; Teichert, C.; Vasic, B.; Matkovic, A.; Ralevic, U.; Gajic, R.; Bayer, B.; Kidambi, P.; Hofman, S, Growth of para-hexaphenyl crystallites on graphene: Nanoscale Pattern Formation at Surfaces. Kopenhagen, Dänmark, 26.05.2013
14. Lechner, R. T.; Popovski, G.; Yarema, M.; Heiss, W.; Armin , H.; Schülli, T.; Paris, O, Chemical and Crystalline Core/Shell Structure of Nanocrystals derived by SAXS/WAXS: 8th European NESY Winter-School & Symposium on Neutrons and Synchrotron Radiation. Planneralm, 8953 Donnersbach, 10.03.2013
15. Lechner, R. T.; Prehal, C.; Burian, M.; Amenitsch, H.; Yarema, M.; Heiss, W.; Paris, O, In-situ synchrotron SAXS studies on Colloidal Nanocrystal Formation: 63. Jahrestagung der Österreichischen Physikalischen Gesellschaft ÖPG 2013., 03.09.2013
16. Lechner, R. T, Der Einfluss der Hüllen-Kristallstruktur auf die optischen Eigenschaften von PbS/CdS Kern-Hülle Nanokristallen: Forum Licht - Green Photonics - Licht für eine energiebewusste Zukunft ., TU Graz, 05.02.2013,
17. Meisels, R, Computational Materials Science in the Nanoworld: On Quantum- Billiards, Carbon Nanostructures and Photonic Crystals: Advanced Simulation of Processes and Phenomena, Montanuniversitaet Leoben., 15.01.2013
18. Nabavi, S.; Hartmann, M, The role of sacrificial bonding on the mechanical properties of polymer chains-a Monte Carlo study: Werkstoffkongress 2013, Montanuniversitaet Leoben, 06.11.2013
19. Nabavi, S.; Matthew J. Harrington, Paris, O.; Peter Fratzl, Hartmann, M, Thermal vibrations reduce the efficacy of sacrificial bonds: DPG Spring Meeting 2013. Regensburg, Germany, 10.03.2013
20. Oesterreicher, A.; Wolfberger, A.; Daschiel, U.; Schmidt, V.; Teichert, C.; Grießer, T, Manufacturing of 3D-Polymer Microstructures via Two-Photon Induced Thiol-Ene Reaction: Photopolymerization Fundamentals 2013 . Jackson / Wyoming (USA), 22.09.2013
21. Paris, O, X-ray and neutron studies of fluids in confinement: TMS annual meeting and exhibition, Symposium: Neutron and X-ray studies of advanced Materials VI: Centennial and Beyond, San Antonio, Texas, USA, March 3th – 7th 2013, 03.03.2013 **(Invited)**
22. Paris, O, Deformation mechanism of nanoporous materials due to phase transitions of fluids and condensed matter in confinement: Biot V Conference on Poromechanics, MS04 Poromechanics of adsorption, Vienna, July 10th – 12th 2013. Vienna, 10.07.2013 **(Invited)**
23. Paris, O, How structural hierarchy determines outstanding performance of biological materials: Contributions from X-ray micro- and nanobeam diffraction: Gordon Research Conference on X-ray Physics, Stonehill College Easton, MA USA, August 4-9, 2013. Stonehill College Easton, MA USA, 04.08.2013 **(Invited)**
24. Sharifi Rajabi, P.; Paris, O.; Marmiroli, B.; Sartori, B.; Cacho-Nerin, F.; Amenitsch, H, Humidity Driven Pore-Lattice Deformation in Ordered Mesoporous Thin Films: Joint Annual Meeting of ÖPG, SPG, ÖGAA und SGAA. Linz, 03.09.2013
25. Sharifi Rajabi, P.; Marlow, F, SANS Analysis of Opal-like Structures made by Capillary Deposition Method (CDM): 8th European NESY Winter- School & Symposium on Neutrons and Synchrotron Radiation, Planneralm (2013). Planneralm, 10.03.2013

26. Teichert, C, Diffusion Mechanisms in the Growth of Organic Semiconductor Nanostructures: 17th International Conference on Crystal Growth and Epitaxy (ICCGE-17), Warsaw, Poland, Aug. 11-16, 2013. Warsaw, Polen, 11.08.2013 **(Invited)**
27. Teichert, C, Graphene as transparent electrode for organic semiconductors: Nano and Photonics, Mauterndorf 2013, Mauterndorf, Austria, March 18 - 22, 2013. Mauterndorf, 18.03.2013, **(Invited)**
28. Teichert, C, Nanoscale Self Assembly Part II (joint With ICN+T 2013) (Session Chair): ICV-19 + ICN + T 2013,Paris, + CNMRS Marseille. Paris, Marseille, Frankreich, 10.09.2013
29. Teichert, C, Graphene as substrate for organic semiconductor thin films: 6th International Workshop on Surface Physics Functional Materials, IWSP, 1-6 September 2013 Niemcza. Institute of Experimental Physics University of Wroclaw, Niemcza, Polen, 02.09.2013
30. Teichert, C, Diffusion Mechanisms in the Growth of Organic Semiconductor Nanostructures: 2013 International Workshop on Nanomaterials and Nanodevices, Beijing, China, July 2013. Beijing, China, 02.07.2013 **(Inited Plenary lecture)**
31. Teichert, C, Exploring what holds paper together: An AFM based nanomechanical investigation of single cellulose fibers and fiber-fiber bonds: ICV-19 + ICN + T 2013 (IVC-19 / ICN+T 2013 and partner conferencesParis, France September 9-13, 2013),Paris, + CNMRS Marseille. Paris, Marseille, Frankreich, 10.09.2013
32. Teichert, C, Wetting and Dewettin Patterns of Dioctylbenzothieno-benzothiophene on Silicon Oxide Surfaces: Int. Symposium on "Nanoscale Pattern Formation at Sufaces", Copenhagen, Denmark 26-30 May, 2013 (Teichert). Copenhagen, 29.05.2013
33. Teichert, C, Session II Chair - Christian Teichert: 6th International Workshop on Surface Physics Functional Materials, IWSP, 1-6 September 2013 Niemcza. Institute of Experimental Physics University of Wroclaw, Niemcza,Polen, 02.09.2013
34. Teichert, C, AFM based characterization of ZnO nanostructures: 2013 International Workshop on Nanomaterials and Nanodevices, Guilin, China, July 2013. Guilin, China, 05.07.2013 **(Invited)**
35. Teichert, C, Atomic Force Microscopy based morphological, electric, and photoelectric characterization of ZnO: International Conference on Oxide-based Materials and Devices (OE108) at SPIE-Photonics West, San Francisco, CA, Feb. 2-7, 2013. San Francisco,CA, USA, 02.02.2013 **(Invited)**
36. Teichert, C, Atomic-force microscopy based diagnostics of functional nanomaterials: International Workshop “Functional Nanomaterials and Devices for Electronics, Sensors and Energy Harvesting”, Kyiv, Ukraine, Apr. 8-11, 2013. Kyiv ,Ukraine, 08.04.2013 **(Invited)**
37. Teichert, C, AFM Based Investigation of Oganic Semiconductor Nanostructures Grown on Graphene Electrodes: Int. Conf. on Metallurgical Coatings & Thin Films ICMCTF 40th Anniversary, April 28-May 3, 2013 San Diego, California (Teichert). San Diego, California, USA, 29.04.2013
38. Teichert, C, Peculiarities in the growth of small organic molecules on graphene substrates: 12th International Conference on Atomically Controlled Surfaces, Interfaces and Nanostructures (ACSIN-12), Tsukuba, Japan, Nov. 4-8, 2013. Tsukuba, 04.11.2013 **(Invited)**
39. Teichert, C, Chair: International Workshop on Nanomaterials and Nanodevices, Beijing, China, July 2013. Beijing, China, 02.07.2013 **(Invited) Chair**
40. Wolfberger, A.; Grießer, T.; Daschiel, U.; Petritz, A.; Fian, A.; Schmidt, V.; Jerrar, A.; Teichert, C.; Kern, W, Photoinduced Cross-linking of Polynorbornenes for 3D Microstructuring and Applications in Organic Electronics: ASPM 2013. Bled, Slowenien, 03.04.2013

Invited talks at external institutions: Seminars 2012/2013

1. Lechner, R. T., Embedded and Colloidal Functional Nanoparticles: Structural Impact on Magnetism and Optics, Seminar - on structure analysis at the Department of Condensed Matter Physics., Charles University Prague, Tchechien, 11.10.2012
2. Lechner, R. T., Colloidal Functional Nanoparticles and Nanocrystal Solids: Structural Impact on Magnetism and Optics, Seminar aus Halbleiter- und Festkörperphysik ., Johannes Kepler Universität, Linz, 12.11.2012

3. Lorbek, S.; Shen, Q.; Teichert, C.; Nabok, D.; Puschnig, P.; Biddau, G.; Draxl, C.; Potocar, T.; Winkler, A., Shape investigations of second-layer islands of para-sexiphenyl thin films on ion-bombarded mica and silicon dioxide substrates & Oblique incidence deposition of para-sexiphenyl thin films on silicon dioxide substrate, NFN Final Project Meeting Leoben. Leoben, 18.01.2012
4. Nevosad, A., Microstructural characterization of ZnO Varistor ceramics, Seminar at Mesa+. University of Twente / Enschede, Niederlande, 22.06.2012
5. Nevosad, A.; Hofstätter, M.; Auer, C.; Piber, M.; Supancic, P.; Teichert, C., Microstructural characterization of ZnO Varistor ceramics, Electroceramics 13. University of Twente / Enschede, Niederlande, 24.06.2012
6. Paris, O., Biomimetic Materials Research: Nature as Source and Inspiraration for Novel functional Materials, Seminar, Institut für Feskörperphysik, TU Graz, 30.05.2012
7. Paris, O., PhysioNanoAkt: Hierarchically structured porous sensor and actuator systems for medical applications, HTI:SMapp project presentation, Land Steiermark, Graz, 22.11.2012
8. Shen, Q.; Lorbek, S.; Kratzer, M.; Pavitschitz, A.; Teichert, C., Characterization of organic thin films by transverse shear and friction force microscopy, NFN Final Project Meeting Leoben. Leoben, 18.01.2012
9. Teichert, C., Advanced atomic-force microscopy based nanostructure characterization, Seminar, Max-Planck-Institut für Eisenforschung. Düsseldorf, Germany, 10.01.2012
10. Teichert, C., What does paper hold together? - An AFM base exploration, Seminar, Institute of Physics of Interfaces and Nanostructures. University of Twente, Enschede, Niederlande, 12.01.2012
11. Teichert, C., Electrical characterization of semiconductor nanostructures, Seminar, Oak Ridge National Lab, Oak Ridge,Tennessee, USA, , April 27. Oak Ridge, Tennessee, USA, 27.04.2012
12. Teichert, C., Step-edge barriers and nucleation in organic thin folm growth, Physikalisches Kolloquium, Osnabrück, Deutschland, June 14, 2012. Osnabrück, 14.06.2012
13. Teichert, C., Atomic force microscopy based nanostructure research, Seminar, Institute of Physics, Jagieelonian University, Krakow, Poland, 14.09.2012
14. Teichert, C., Graphene as substrate for organic semiconductor thin film, Seminar, Max Planck-Institut für Mikrostrukturphysik, Halle/Saale, Deutschland, Nov. 15, 2012. Halle/Saale, 15.11.2012
15. Teichert, C., Graphen als Substrat für organische Halbleiterschichten, Physikalisches Kolloquium, Technische Universität Illmenau, Deutschland, 20.11.2012
16. Teichert, C., Conductive Atomic Force Microscopy Investigation of Nanostructures in Microelectronics, Seminar, Fraunhofer-Center für Silizium Photovoltaik CSP, Halle/Saale,Deutschland, 21.11.2012
17. Teichert, C., Organic semiconductor thin films explored by AFM based techniques, Seminar aus nano- und Quantenphysik, Department Physik, Universität Basel, Switzerland, 03.12.2012
18. Ganser, C., Atomic force microscopy based methods for mechanical characterization of cellulosic materials, Seminar Festkörperphysik 2, Technische Universität Graz, 13.03.2013
19. Ganser, C.; Schmied, F.; Fischer, W.; Hirn, U.; Schennach, R.; Teichert, C, Mechanical characterization of pulp fibers by atomic force microscopy based methods: Nanobrücken Dresden. Technische Universität Dresden, Germany, 20.03.2013
20. Kratzer, M, The atomic force microscope as versatile tool in surface characterization and manipulation : Solid State Institute Seminar. Graz University of Technology, 16.10.2013
21. Kratzer, M, Modification of exfoliated graphene: an AFM study: Seminar am MPI for Polymer Research. Max Planck Institute for Polymer Research, Germany, 27.11.2013
22. Lechner, R. T, Embedded Nanostructures and Core/Shell Colloidal Nanocrystals: How Structure Determines Magnetism and Optics, Seminar aus Festkörperphysik, Institut für Physik, KFU Graz, 07.01.2013
23. Lechner, R. T, Combining SAXS/WAXS Studies with Complementary Techniques for Detailed Characterisations of Diluted and Densely Packed Nanocrystals, Special Seminar on Inorganic Nanostructures. Laboratory of Inorganic Chemistry, ETH Zürich, Switzerland, 19.11.2013
24. Oswald, J., Quantum Electron Transport in high Magnetic Fields, 8 hours seminar course 25.2. – 9.3.2013 at the Graduate school of science, Physics Department, Chiba University, Japan
25. Paris, O, Synchrotronstrahlung zur Charakterisierung komplexer nanomaterialien, Kolloquium anorganische Chemie, TU München, 14.01.2013.

26. Paris, O, Synchrotron radiation studies of complex biological and bioinspired materials: School of Engineering and Materials Science, Queen Mary University of London, 28. February 2013. London, United Kingdom, 28.02.2013
27. Paris, O., Biomimetic Materials Research: Nature as Source and Inspiraration for Novel functional Materials, Seminar, Institut für Feskörperphysik, TU Graz, 30. May 2012
28. Teichert, C, Exploring organic thin film growth on graphene by LEEM and AFM: Condensed Matter Physics Seminar, University of California Davis, California Davis, USA, 30.01.2013
29. Teichert, C, Exploring organic thin films by atomic-force microscopy based techniques: Seminar at the Foundry, Lawrence Berkely Laboratory, Berkely, CA, USA, 01.02.2013
30. Teichert, C, Graphene as substrate for organic semiconductor thin films: Seminar, Sino-German College, East Chinese University of Science and Technology, Shanghai, China, 15.03.2013
31. Teichert, C, Growth of small organic molecules on graphene: Festkörperphysik-Seminar, KFU Graz, (April 15). KFU Graz, 05.04.2013
32. Teichert, C, Introducing graphene substrates to organic thin film growth: Seminar, Institute of Physics, National Academy of Sciences of Ukraine, Kiev, Ukraine, 12.04.2013
33. Teichert, C, Electric and photoelectric characterization of freestanding ZnO nanowires: Seminar on Condensed Matter Physics, Dept. of Physics, Simon Fraser University, Burnaby, BC; Canada, 01.05.2013
34. Teichert, C, Growth of organic thin films on graphene substrates: Seminar CINAM-CNRS Marseille, France, Marseille, Frankreich, 16.09.2013
35. Teichert, C, Morphological and nanomechanical investigation of single cellulose fibers and fiber-fiber bonds using atomic-force microscopy: Advanced Materials Seminar, LIOS, JKU Linz, 04.10.2013
36. Teichert, C, Atomic-force microscopy based exploration of cellulose fibers and their bonds: TUG/KFU Physics Colloquium, TU Graz, 15.10.2013
37. Teichert, C, Graphene as substrate for small organic molecules: Seminar, Japan Institute of Science and Technology, Ishikawa, Japan, 11.11.2013

Posters 2012

1. Ganser, C.; Schennach, R.; Teichert, C.,Investigations of cellulose fibers in water by atomic force microscopy, XIV. Annual Linz Winter Workshop. Linz, Österreich, 03.02.2012
2. Ganser, C.; Schennach, R.; Teichert, C., AFM investigation of kraft pulp fiber swelling in controlled humidity, 62. Jahrestagung der Österreichischen Physikalischen Gesellschaft. Graz, Österreich, 18.09.2012
3. Ganser, C.; Schmied, F.; Schennach, R.; Hirn, U.; Teichert, C., Atomic force microscopy as a tool to characterize single pulp fibers and fiber-fiber bonds, 1st COST Action FP1105 Workshop. Stockholm, Schweden, 03.12.2012
4. Grießer, T.; Wolfberger, A.; Daschiel, U.; Schmidt, V.; Jerrar, A.; Teichert, C.; Kern, W.,Cross-linking of a ROMP Derived Polymer Using the Thiol-Ene Reaction: Towards the Fabrication of Polymer 2D- and 3D-Microstructures, European Symposium on Photopolymer Science. Torino, Italien, 04.09.2012
5. Hofstätter, M.; Nevosad, A.; Auer, C.; Piber, M.; Supancic, P.,Polarity-dependent electrical characteristics of ZnO varistor ceramics, Electroceramics XIII. University of Twente/Enschede,Niederlande, 25.06.2012
6. Kratzer, M.; Klima, S.; Vasić, B.; Gajić, R.; Matković, A.; Ralević, U.; Teichert, C.,Dynamic plowing lithography and 6P thin film growth on graphene investigated by atomic force microscopy, ÖPG 2012. Graz, Österreich 17.09.2012
7. Kratzer, M.; Klima, S.; Vasić, B.; Gajić, R.; Matković, A.; Ralević, U.; Teichert, C.,Growth of para-hexaphenyl thin films on graphene:an AFM study, ElecMol2012. Grenoble, Frankreich, 03.12.2012
8. Kreiml, P.; Ganser, C.; Schennach, R.; Teichert, C.,Morphological investigations of viscose fibers by atomic force microscopy, 62. Jahrestagung der Österreichischen Physikalischen Gesellschaft. Graz, Österreich, 18.09.2012
9. Lechner, R. T.; Zizak, I.; Yarema, M.; Primorac, M.-M.; Heiss, W.; Paris, O.,Crystal structure of self assembled micron sized colloidal nanocrystal solids investigated in the SAXS and WAXS regime, 15th International Small-Angle Scattering Conference 2012 (SAS2012). Sydney, Australien, 18.11.2012

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11. Nabavi, S.; Harrington, M. J.; Fratzl, P.; Hartmann, M.,The influence of sacrificial bonds on cyclic loading of a single polymer chain - A Monte Carlo simulation study, Bio-inspired Materials. Potsdam, 20.03.2012
12. Nevosad, A.; Hofstätter, M.; Supancic, P.; Teichert, C.,Microscopical investigation of grain boundaries in ZnO varistor ceramics, Jahrestagung der ÖPG 2012. Graz, Österreich, 18.9.2012
13. Nabavi, S.; Hartmann, M.,The effect of sacrificial bonds on the mechanical behavior of a polymer chain-A Monte Carlo simulation study, The 62nd Annual Mee ting ÖPG 2012. Graz, Österreich, 18.09.2012
14. Oswald, J.; Uiberacker, C.,Numerical simulations of scanning gate experiments in the quantum Hall effect regime, 17th International Winterschool on New Developments in Solid State Physics. Mauterndorf, Salzburg, Österreich, 12.02.2012
15. Oswald, J.; Uiberacker, C.,Numerical simulations of scanning gate experiments in the quantum Hall effect regime, 62. Jahrestagung der Österreichischen Physikalischen Gesellschaft, Graz, Österreich, 18.09.2012
16. Popovski, G.,Two Dimensional Indirect Fourier Transformation, SAS 2012. Sydney, 11.11.2012
17. Rebelo De Figueiredo, M.; Bergmann, C.; Ganser, C.; Teichert, C.; Mitterer, C.,Adhesion of polymers to hard coatings, ICMCTF 2012. San Diego /USA, 23.04.2012
18. Teichert, C., Characterisation of nanostructures induced by slow highly charged ion bombardment of HOPG, 25th Intern. Conf. on Atomic Collisions in Solids (ICACS-25), Kyoto University, Kyoto, Japan, 23.10.2012. Kyoto, Japan, 23.10.2012
19. Wrana , D.; Kratzer, M.; Teichert , C.; Krok, F.,Wzrost molekul para-sexiphenylu na zmodykowanej wiazka jonowa powierzchni TiO_2 (110), Polish Scanning Probe Society Meeting VII Seminarium STM/AFM 2012. Zakopane, Poland, 28.11.2012

Posters 2013

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2. Burian, M.; Yarema, M.; Popovski, G.; Amentisch, H.; Heiss, W.; Paris, O.; Lechner, R.,Shape Retrieval from Colloidal Nanocrystals by SAXS, Research at European Neutron and Synchrotron facilities by Austrian resarchers. Vienna University of Technology, Österreich, 11.11.2013
3. Ganser, C.; Schmied, F.; Schennach, R.; Teichert, C.,Atomic force microscopy based methods to study mechanical properties of cellulose fibers, 2013 MRS Spring Meeting. San Francisco, California, USA, 01.04.2013
4. Mirkowska, M.; Kratzer, M.; Teichert, C.; Flachberger, H.,Kelvin probe force microscopy investigations of the contact charging of single crystalline insulators, Annual Meeting of German Physical Society (DPG) . Regensburg, Germany, 12.03.2013
5. Mirkowska, M.; Kratzer, M.; Teichert, C.; Flachberger, H.,Charge behavior on insulating monocrystallic surfaces by Kelvin probe force microscopy, Annual Meeting of Austrian Physical Society (ÖPG). Linz, Austria, 03.09.2013
6. Mirkowska, M.; Kratzer, M.; Teichert, C.; Flachberger, H.,Charging behavior of the calcite (100) surface investigated by KPFM, 1st French-German Summer School on noncontact atomic force microscopy. Porquerolles, France, 06.10.2013
7. Morak, R.; Popovski, G.; Van Opdenbosch, D.; Zollfrank, C.; Paris, O., Structure and sorption analysis of wood templated ceramic, 8th European NESY Winter-School & Symposium on Neutrons and Synchrotron Radiation. Planneralm, Österreich, 10.03.2013
8. Morak, R.; Popovski, G.; Van Opdenbosch, D.; Zollfrank, C.; Paris, O.,Hierarchical biotemplating in nanometer scale, Research at European Neutron and Synchrotron facilities by Austrian researchers. Wien, Österreich 11.11.2013
9. Nabavi, S.,The density and distribution of sacrificial bonds in polymer chains determines the amount of dissipated energy, ÖPG Jahrestagung 2013, Linz, Österreich, 02.09.2013

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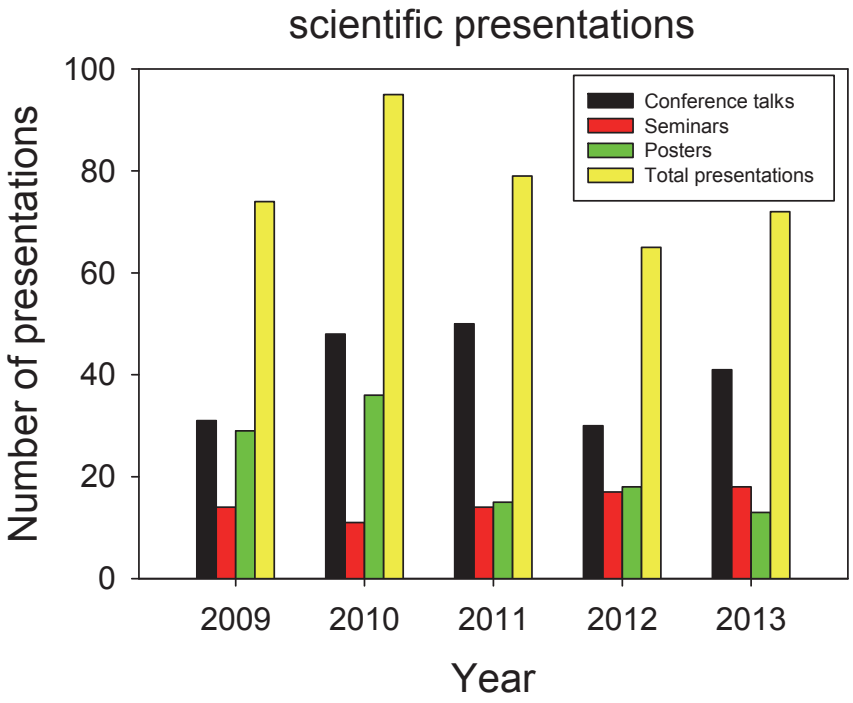
11. Sharifi Rajabi, P.; Marmiroai, B.; Sartori, B.; Cacho-Nerin, F.; Amenitsch, H.; Ganser, C.; Teichert, C.; Paris, O.,Humidity Driven Pore- Lattice Deformation in Ordered Mesoporous Thin Films, Research at European Neutron and Synchrotron facilities by Austrian researchers, Vienna (2013). Vienna, Österreich, 11.11.2013
12. Sharifi Rajabi, P.; Marmiroai, B.; Sartori, B.; Cacho-Nerin, F.; Amenitsch, H.; Ganser, C.; Teichert, C.; Paris, O.,Humidity Driven Pore- Lattice Deformation in Ordered Mesoporous Thin Films, MRS fall meeting, Boston, 01.12.2013
13. Wolfberger, A.; Petritz, A.; Fian, A.; Stadlober, B.; Schmidt, V.; Teichert, C.; Grießer, T.,Photolithographic Patterning of Polynorbornenes: Towards Applications in Optics and Organic Electronics, Swiss ePrint 2013. Basel, Schweiz, 21.11.2013



Awards 2012/2013

- **Roland Brunner**: Förderungspreis des Landes Steiermark 2012 for the paper: ,,Two-Qubit Gate of Combined Single-Spin Rotation and Interdot Spin Exchange in a DoubleQuantum Dot"
- **Franz Schmied**: "Best Presenter Award"; International Paper Physics Conference, 13. June 2012 in Stockholm
- **Reinhold Wartbichler**: “Best Poster Prize” Joint Annual Meeting of the Austrian and the Swiss Physical Society, Linz, 3.-6.9.2013.
- **Tomas Kamencek**: Second Prize of the Best Physics Paper of Austrian High School students 2012 for his experimental work in the Scanning Probe Microscopy Group of the institute.
- **Roland Morak**: Leistungsstipendium for students of the MUL 2012/2013
- **Christian Prehal**: Leistungsstipendium for students of the MUL 2012/2013
- **Max Burian**: Förderungsstipendium for students of the MUL 2012/2013
- **Christian Prehal**: Förderungsstipendium for students of the MUL 2012/2013

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 30 Jun.2015
Project leader:	M. Hartmann
Coworker(s):	S.Nabavi
Funding:	€ 141.000,--

Project:	**"Exploring fundamental growth morphologies in organic thin film systems"**
Funded by:	FWF within the National Research Network "Interface controlled and functionalized organic films" (S9707-N20)
Start:	1 Feb 2009
Duration:	until 31 Aug 2012
Project leader:	C. Teichert
Coworker(s):	S. Lorbek, Q. Shen
Funding:	€ 212.248,--

Project:	**"Microwave-induced modifications of thermal and mechanical properties of rocks and their consequences for rock fragmentation**"
Funded by:	FWF (TRP 284-N30 Translational-Research-Program)
Start:	1 April, 2013
Duration:	until 31 March, 2016
Project leader:	T. Antretter (Institut für Mechanik)
Co-Applicant:	F. Kuchar
Funding:	€ 70.000,-- (inkl. 20% Gemeinkosten)

Project:	**"Bridging length scales to analyse and enhance the performance of piezoceramics for commercial actuators"**
Funded by:	FWF(TRP 302-N20)
Start:	1.9. 2013
Duration:	until 31 Aug 2016
Project leader:	M. Deluca
Co-Applicant	C.Teichert
Coworker(s):	M. Kratzer, M. Lasnik
Funding:	€ 27.500,--

§ 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
Project leader	O. Paris
Coworker(s)	G. Popovski, R. Morak
Funding:	€ 165.000,--

Project:	**“Hierarchische poröse Sensorsysteme zur *in-vivo* Detektion von Änderungen des physiologischen Umgebungsmilieus in der Humanmedizin”**
Funded by	Land Steiermark: Human Technology Interface: Sensors for medical applications (HTI:SMapp)
Start	1. Sept 2012
Duration	until 31. May 2014
Project leader	O. Paris
Coworker(s)	P. Sharifi, C. Prehal, M. Burian, C. Ganser, C. Teichert
Funding:	€ 140.000,--

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
Project leader:	Christian Teichert
Coworker(s):	M. Kratzer, A. Nevosad (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
Project leader:	R. Meisels
Coworker(s):	O. Glushko, R. Brunner
Funding:	€ 200.286,--

Participation in CD Laboratories

Project:	**CD Labor Papierfestigkeit**
Funded by:	Christian Doppler Gesellschaft
Start:	1. Jan 2007
Duration:	31. Aug 2014
Project leader:	R. Schennach, TU Graz
Co-Project leader	C. Teichert
Coworker(s):	C. Ganser, P. Kreiml, C. Czibula
Funding:	€ 300.000,--

Other Projects

Project:	**“Eindimensionale molekulare Selbstorganisation auf Siliciumtemplaten”**
Funded by:	ÖAD/ Wissenschaftlich-Technisches Abkommen mit Frankreich, Amadee 2013-2014 (FR 17/2003)
Start:	1 Jan 2013
Duration:	until 31 Dec 2014
Project leader:	C. Teichert
Co-Applicant:	L. Masson, Institut CINAM-CNRS, Campus Luminy, Marseille France
Coworker(s):	M. Kratzer, M. Mirkowska, S. Klima, A. Nevosad (Pavitschitz
Funding:	€ 5.950,--

Project:	**"Elektrische und mechanische Eigenschaften von organischen Dünnschichten auf der Nanometer-Skala"**
Funded by:	ÖAD/ Wissenschaftlich-Technisches Abkommen mit Polen, 2012-2013 (PL19/2012)
Start:	1 April 2012
Duration:	until 31 March 2013
Project leader:	C. Teichert
Co-Applicant:	F. Krok, Institute of Physics, Jagiellonian University, Krakow
Coworker(s):	M. Kratzer, M. Mirkowska, R. Wartbichler, M. Klima
Funding:	€ 6000,--

Project:	**"Morphologie, Transport und photovoltaische Eigenschaften niedrigdimensionaler Heterostrukturen für Solarzellenanwendungen"**
Funded by:	ÖAD/ Wissenschaftlich-Technisches Abkommen mit der Ukraine, 2013-2014 (UA 11/2013)
Start:	1 Jan 2013
Duration:	until 31 Dec 2014
Project leader:	C. Teichert
Co-Applicant:	S. Kondratenko, Taras Shevchenko Naio9nalUniversiy of Kyiv,Phsics Departmen, Optics Division, Kiev, Ukraine
Coworker(s):	M. Kratzer, M. Mirkowska, C. Ganser, C. Czibula
Funding:	€ 6.029,--

Project:	**"Piezoelektrische Energiewandler auf Basis von vertikal ausgerichteten Nanokristallen: Herstellung und Charakterisierung geodneter Nanostab-Anordnung"**
Funded by:	ÖAD/ Wissenschaftlich-Technisches Abkommen mit der Ukraine, 2013-2014 (UA 05/2013)
Start:	1 Jan 2013
Duration:	until 31 Dec 2014
Project leader:	M. Kratzer
Co-Applicant:	O. Dimitriev, V. Lashkaryov Insitute of Semiconductor Physics, Kiev, Ukraine
Coworker(s):	M. Mirkowska, S. Klima, A. Nevosad (Pavitschitz)
Funding:	€ 5.604,--

Funded experimental measurement time at large scale facilities

In addition to funded projects from national and international funding agencies, the Institute of Physics is also very active in acquiring measurement time for experimental work at large scale facilities. The allocation of measurement time requires submitting a proposal for the planned experiment, which is then reviewed by an international panel and beamtime is granted on the basis of scientific excellence. Within the reporting period, we were able to get 7 beamtimes at synchrotron radiation facilities, one beamtime at a neutron radiation facility and one measurement time at a Scanning Probe Microscopy facility. All in all, 58 days of beamtime were granted to the Institute.

Year	Main proposer	Co-proposer(s)	Titel of Proposal	Facility	Measuring days
2012	M. Erko	O. Paris (MUL)	Water in Confined Geometry	FRMII-München	10
	R.T. Lechner	G. Popovski, O. Paris (MUL)	Anomalous WAXS studies of core/shell nanocrystals	ESRF-Grenoble	5
	R.T. Lechner	G. Popovski, O. Paris (MUL)	Anomalous SAXS and WAXS studies of PbS/CdS core-shell nanocrystals	HZB-BESSY Berlin	3
	R.T. Lechner	O. Paris (MUL)	In-situ investigation of the self-assembled growth of nanocrystal solids with SAXS	ELETTRA-Triest	6
					24
2013	O. Paris	P. Sharifi, R. Morak (MUL); H. Amenitsch, B. Marmiroli, B. Sartori (TU Graz); E. Martinelli, A. Weinberg (Med. Uni Graz)	Deformation of ordered mesoporous materials due to protein adsorption	ELETTRA-Triest	6
	O. Paris	P. Sharifi (MUL); H. Amenitsch, B. Marmiroli, B. Sartori (TU Graz)	Deformation of ordered mesoporous thin films due to water adsorption and condensation	ELETTRA-Triest	6
	O. Paris	C. Prehal, R.T. Lechner (MUL); V. Presser, E. Perre, J. Atchison (INM Saarbrücken)	In-situ SAXS Studies on the Charge/Discharge Behavior of Electrochemical Double layer Capacitors	ELETTRA-Triest	6
	O. Paris	P. Sharifi, R. Morak (MUL); H. Amenitsch, B. Marmiroli, B. Sartori (TU Graz)	Deformation of ordered mesoporous thin films due to water adsorption and condensation: The influence of film thickness and film perfection	ELETTRA-Triest	6
	C. Teichert	A. Nevosad, P. Supancic (MUL), S. Kalinin, E. Strelkov (CNMS, Oak Ridge, National Lab.)	Scanning probe microscopy based investigation of ZnO varistor ceramics	CNMS, Oak Ridge, National Lab.	10
					34

7. Diploma and Doctoral Theses

7.1 Diploma Theses

Patrice KREIML Supervisor: C. Teichert Since: Dec 2013	Investigation of water absorption of cellulose fibers by atomic force microscopy and gravimetric analysis
Caterina CZIBULA Supervisor: C. Teichert Since: Sept 2013	Roughness analysis and chemical contrast of cellulose model films studied by atomic force microscopy
Lin WANG Supervisor: C. Teichert Finished: Mar 2012	Conductivity investigation on ZnO nanorods using atomic-force microscopy
Max BURIAN Supervisors: O. Paris, R.T. Lechner Finished: May 2014	Shape retrieval of inorganic nanocrystals from SAXS-data
Christian PREHAL Supervisor: O. Paris Finished: Feb 2014	In-Situ SAXS study on the ion dynamics in microporous carbon based supercapacitors
Roland J. MORAK Supervisor: O. Paris Finished: Jun 2013	Structure and sorption analysis of wood templated ceramics
Mario LUGGER Supervisor: C. Teichert Finished: Feb 2012	Friction reduction between polymer and injection mold surface: Influence of surface roughness on surface energy and interfacial tension

7.2 Doctoral Theses

Roland J. MORAK Supervisor: O. Paris Since: Oct 2013	Sorption induced deformation of materials with hierarchical porosity
Seyedsoran NABAVI Supervisors: O. Paris & M. Hartmann Since: Oct 2011	Understanding Interfaces in Biological Tissue
Christian GANSER Supervisor: C. Teichert Since: Oct 2011	Influence of water on mechanical properties of cellulosic materials studied by AFM based methods
Quan SHEN Supervisor: C. Teichert Since: Jun 2009	Atomic-force microscopy based characterization on functionalized organic thin films
Stefan LORBEK Supervisor: C. Teichert Since: Jan 2009	Molecular processes in organic thin film growth

Maxim ERKO Supervisor: O. Paris Finished: March 2012	Water properties in confined geometry
Andreas NEVOSAD (PAVITSCHITZ) Supervisor: C. Teichert Finished: Oct 2013	Conductive probe based investigations on ZnO varistor ceramics

8. Incomings: Invited Guests (Seminar)

2012

	Kolloquium zu den Nobelpreisen 2013
Thu, 13. December 2012 (gemeinsam mit dem Department Allgemeine Analytische und Physikalische Chemie, Technologieakademie und Materials Cluster Styria)	O.Univ.-Prof. Dr. Helmut Rauch *(Atominstitut, Technische Universität Wien)* **„Quantenphysik macht Furore“** Der Nobelpreis für Physik 2012 geht an zwei Pioniere der Quantenoptik, an den Franzosen **Serge Haroche** vom Collège de France und der École Normale Supérieure in Paris sowie an **David Wineland** vom National Institute of Standards and Technology und der University of Boulder, USA, für die „bahnbrechenden experimentellen Verfahren, die es erlauben Quantensysteme zu messen und zu manipulieren“. Univ.-Prof. Dr. Klaus Richter *(Fachbereich Zellbiologie, Universität Salzburg)* **„G-Protein gekoppelte Rezeptoren – unübertroffen in der Signalübertragung**“ Der Nobelpreis für Chemie 2012 geht an die beiden US-Wissenschafter **Robert Lefkowitz** vom Howard Hughes Medical Institute and Duke University Medical Center, Durham, USA und **Brian Kobilka** von der Stanford University School of Medicine, USA, für deren Entdeckungen über die Funktionsweise von G-Protein gekoppelten Rezeptoren.
Thu, 13. December 2012	Prof. Dr. Franciszek Krok *(Institute of Physics, Jagiellonian University, Krakow, Poland)* **"Temperature dependent rotation of self-organised nanopatterns on ion-irradiated TiO2(110)“**
Tue, 4. December 2012	Univ.Prof. Dr. Roland Resel *(Institut für Festkörperphysik, TUGraz)* **„Buried interfaces in organic electronic devices: x-ray reflectivity studies“**
Tue, 27. November 2012	Prof. Dr. Christoph Tegenkamp *(Institut für Festkörperphysik, Leibniz, Universität Hannover, Germany)* **“The phenomenon of contact charging - fundamentals and applications**
Tue, 13. November 2012	Dr. Bernd Dittert , Dr. Michael Mühlberger (*Functional Surfaces and Nanostructures,* PROFACTOR GmbH, Steyr) **“Nanoscaled oxides: Patterning of thin films and particle synthesis”**
Tue, 30. August 2012	Dr. Himadri S. Gupta *(Lecturer in Biomaterials School of Engineering and Materials Science Queen Mary University of London, Mile End Road, London , UK)* **"Nanostructural Mechanisms of Mineralized Tissue Toughness and Their Modification in Metabolic Bone Disease"**

Tue, 28. August 2012 Dr. Volker Presser
(Head of Energy Materials Group, INM Leibniz-Institut für Neue Materialien gGmbH, Saarbrücken, Germany)
"Novel and Hierarchical Carbon Nanomaterials for Energy-Related Applications"

Tue, 26. June 2012 Ao.Univ.Prof. Dr. Robert Schennach
(Institute of Solid State Physics, Graz University of Technology, CD-Laboratory for Surface Chemical and Physical Fundamentals of Paper Strength, Graz)
"A surface science view on paper – the unnoticed high tech material"

Tue, 12. June 2012 Univ.Prof. Dr. Günther Bauer
(Institut für Halbleiter- und Festkörperphysik, Universität Linz)
"Silicon-Germanium Alloys: From Physics to Applications"

Tue, 5. June 2012 Univ.Prof. Dr. Walter Pötz
(Institut für Theoretische Physik, Karl Franzens Universität Graz)
"Ways for Coupling Spin to Charge: Examples from Solid-State"

Tue, 15. May 2012 Prof. Dr. Václav Holý
(Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University in Prague, Praha, Czech Republic)
"STRUCTURE OF EPITAXIAL LAYERS OF DILUTED FERROMAGNETIC SEMICONDUCTORS INVESTIGATED BY X-RAY RELATED METHODS"

Tue, 8. May 2012 Univ.Prof. Dr. Herwig Peterlik
(Faculty of Physics, University of Vienna)
"Small-angle X-ray scattering as a method to follow nanostructures and evolution of nanostructures in-situ"

Mon, 7. May 2012 Prof. Dr. Radoš Gajic
(Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade)
"Optical Spectroscopy of Single and Few-Layer Graphene"

Thu, 19. April.2012 Dr. Christian Hagendorf
(Fraunhofer Institut, Halle, Germany)
"Classification and Investigation of Recombination Active Defects in Multicrystalline Silicon Thin Film Solar Cells"

Wed, 18.4.2012 Dr. Gudrun Reichenauer
(Bayerisches Zentrum fuer Angewandte Energieforschung e.V. Abt. Funktionsmaterialien der Energietechnik, Bavarian Center for Applied Energy Research, Würzburg, Germany)
"Erhöhung der Energieeffizienz durch Einsatz nanoporöser Materialien - von den Grundlagen zur Anwendung"

Tue, 3. April 2012 Prof. Dr. David J. Dunstan
(School of Physics and Astronomy, Queen Mary, University of London, U.K.)
"Solvent and pressure effects on carbon nanotubes"
*Zusammen mit dem **Erich Schmid Kolloquim,** Institut für Materialphysik und Erich Schmid Institut für Materialwissenschaft der Österreichischen Akademie der Wissenschaften*

Tue, 13. March 2012 Dr. Franz Zerobin
(*Tridonic Jennersdorf GmbH, Jennersdorf)*
"Status und Herausforderungen von LED's in der Lichttechnik"

Thu, 1. March 2012	Dr. Gregor Hlawacek *(Faculty of Science and Technology, Physics of Interfaces and Nanomaterials (PIN), University of Twente, Enschede, The Netherlands)* **"The UHV Helium Ion Microscope - Imaging ultra-thin layers with ions"**
Tue, 28. February 2012	Dr. Harald Reichert, *(wissenschaftlicher Direktor der Europäischen* Synchrotronstrahlungsquelle ESRF) **"Science with Synchrotron Radiation from a 6 GeV"**
Tue, 31. January 2012	Prof. Dr. Ernst Meyer *(Universität Basel, Schweiz)* **"Atomic friction"**
Tue, 24. January 2012	Prof. Dr. Gunter Springholz *(Johannes Kepler Universität Linz)* **„In situ growth studies of SiGe growth on pre-patterned and high-indexed vicinal Si Substrates"**

2013

	Kolloquium zu den Nobelpreisen 2013
Thu, 12. December 2013 (gemeinsam mit dem Department Allgemeine Analytische und Physikalische Chemie, Technologieakademie und MATERIALS CLUSTER STYRIA	ao.Univ.-Prof. Dr. Michael Ramek *(Institut für Physikalische und Theoretische Chemie, Technische Universität Graz)* „Taking the Experiment to Cyberspace" - Zum Nobelpreis für Chemie 2013 Der Nobelpreis für Chemie 2013 geht an drei US-Wissenschafter mit ganz unterschiedlichen Wurzeln: an **Martin Karplus** (geboren in Wien), an **Michael Levitt** (geboren in Pretoria) und an **Arieh Warshel** (geboren im Kibbuz Sde Nahum) für die **„Entwicklung von Multiskalenmodellen für komplexe chemische Systeme".** Privatdoz. Dr. Manfred Jeitler *(Institut für Hochenergiephysik der Österreichischen Akademie der Wissenschaften, Wien)* **„Das Higgs-Boson: lange gejagt, endlich gefunden!"** Der Nobelpreis für Physik 2013 geht an **Francois Englert** (Belgien) und **Peter Higgs** (Schottland) für die theoretische Vorhersage des Higgsteilchens, welches 2012 durch zwei Experimente am Large Hadron Collider des CERN nachgewiesen werden konnte. Damit wurde der letzte, seit Jahrzehnten intensiv gesuchte Bestandteil des so genannten Standardmodells der Elementarteilchen gefunden.
Tue, 10. December 2013	Dr. Luca Bertinetti *(Max Planck Institute of Colloids and InterfacesDepartment of Biomaterials, Potsdam, Germany)* **"Wood swelling with humidity: an EOS approach using the concept of force balance"**
Tue, 3. December 2013	Dr. Heinz H. Busta *(University of Illinois at Chicago und Prairie Prototypes, LLC)* **"The future of microelectromechanical systems (MEMS) and the role graphene might play"**
Tue, 26. November 2013	Dipl.Ing. Andreas Nevosad *(Institute of Physics, Montanuniversitaet Leoben)* **"Conductive probe based investigations on ZnO varistor ceramics"**

Tue, 29. Oktober 2013	Dr. Eugene Bortchagovsky *(Inst. of Semiconductor Physics of the Ukrainian Academy of Sciences, Kiev)* **"SNOM + SERS = TERS and how functionalized tips can improve this equation"**
Tue, 22. Oktober 2013	Univ.- Doz. Mag. Dr. Anton Köck *(Materials Center Leoben Forschung GmbH (MCL) Leoben)* **„Metal Oxide Nanowire Gas Sensors for Indoor and Outdoor Environmental Monitoring"**
Fri, 2. August 2013	Dr. Andrei L. Kholkin *(Department of Materials and Ceramics Engineering and Center for Research in Ceramic and Composite Materials (CICECO), University of Aveiro, Portugal)* **"Nanoscale piezoelectricity of functional materials: from oxides to bioinspired nanotubes and tissues**"
Tue, 9. Juli 2013	Prof. Dr. Gerhard Findenegg *(Stranski Laboratorium für Physikalische und Theoretische Chemie, TU Berlin)* **"Tenside und Proteine in Wechselwirkung mit nanoskaligen Silica-Materialien"**
Tue, 18. Juni 2013	Ass. Prof. Dr. Alois Lugstein *(Institut für Festkörperelektronik der TU Wien, Wien)* **"Si and Ge nanowires as building blocks for novel devices"**
Tue, 14. Mai 2013	Prof. Dr. Kurt Hingerl *(Center for surface- and nanoanalytics, University Linz, Austria)* **"Bulk dipole contribution to second harmonic generation in diamond lattices"**
Tue, 12. März 2013	Dr. Herbert Gold *(Joanneum Research, Weiz)* **"Nanoimprint Lithography - Methods and Applications"**
Tue, 22. Jänner 2013	Univ.-Doz. Dr. Georg Pabst, PhD *(Institut für Molekulare Biowissenschaften, Karl Franzens Universität , Graz)* **"Physics of Cellular Communication"**

9. Outgoings: Foreign Research Visits of Institute Members

R. T. Lechner	25.07.2012 - 30.07.2012	Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlungm.b.H.
	02.08.2012 - 08.08.2012	Synchrotron ELETTRA, Sincrotrone Trieste (Italien)
	04.12.2012 bis 11.12.2012	European Synchrotron Radiation Facility - ESRF (Frankreich)
	08.05.2013 bis 15.05.2013	Synchrotron ELETTRA, Sincrotrone Trieste (Italien)

A. Nevodas	07.04.2013 - 14.04.2013	CNMS, Oak Ridge National Lab, Tennessee (USA)
J. Oswald	25.02.2013 bis 09.03.2013	Chiba University (Japan)
O. Paris	06.02.2013 - 11.02.2013	Synchrotron ELETTRA, Sincrotrone Trieste beamtime GI-SAXS (Italien)
G. Popovski	04.12.2012 - 10.12.2012	European Synchrotron Radiation Facility ESRF (Frankreich)
	01.04.2013 - 30.09.2013	Guest Professor: Universität Kassel (Deutschland)
C. Prehal	15.04.2013 - 20.04.2013	SAXS Beamline, Synchrotron ELETTRA Trieste (Italien)
	08.05.2013 bis 14.05.2013	SAXS Beamline, Synchrotron ELETTRA Trieste (Italien)
C. Teichert	12.09.2012 - 16.09.2012	Institute of Physics, Jagellonian University Krakow (Polen)
	31.01.2013 - 07.02.2013	Dept. of Nuclear Engineering, University of California, Berkeley (Vereinigte Staaten (USA))
	03.04.2013 - 07.04.2013	Institute of Physics, Jagellonian University Krakow (Polen)
	08.04.2013 - 13.04.2013	Institute od Physics, Natl. Acad. of Sciences, Kiev Ukraine (Ukraine)
	13.09.2013 - 17.09.2013	CINAM-CNRS Marseille (Frankreich)

10. Conference Organisation

Organisation of Conferences, Workshops or Schools

Oskar Paris
- 10. Werkstoffkongress, Next Generation of Materials and Devices from Bioinspiration, 6th/7th November 2013, Leoben, Austria

Oskar Paris & Rainer T. Lechner
- 8th European NESY Winter-School & Symposium on Neutrons and Synchrotron Radiation including topical highlight lectures on Nanostructured Materials for Applications in Electronics, Magnetics and Spintronics, Planneralm (Austria), March 10-16, 2013, Austria

Friedemar Kuchar, G. Bauer, W. Jantsch
- 17th International Winterschool on New Developments in Solid State Physics, "Mauterndorf 2012", 12 - 17 Feb, 2012, Castle of Mauterndorf, A-5570 Mauterndorf, Province of Salzburg, Austria

Organisation of Symposia or Sessions at Conferences

Oskar Paris
- Condensed Matter Session, Common annual Meeting of the Austrian Physical Society and the Swiss Physical Society (with Peter Hadley, TU Graz & Christian Ruegg PSI Villigen), 3.-6. September 2013, Linz, Austria
- Organisation Committee and Symposium Chair: NESY-Symposium: Research at European Neutron and Synchrotron Facilities by Austrian Scientists", TU Wien, Nov. 11th/12th 2013

Christian Teichert
- Surfaces, Interfaces and Thin Films Section, Annual Meeting Austrian Physical Society, Graz, Sept. 18-21, 2012
- Surfaces, Interfaces and Thin Films Section, Common annual Meeting of the Austrian Physical Society and the Swiss Physical Society, 3.-6. September 2013, Linz, Austria
- Member of Scientific Committee "Third European Workshop on Self-organized Nanomagnets, Guadarrama, Spain, Apr 16-20 2012.
- Member of the International Steering Committee und Program Committee, Intl. Conference on Nanoscience + Technology (ICN+T 2012), Paris, July 23-27, 2012.
- Symposium Chair "Graphene and 2D nanostructures", ICMCTF 2013, San Diego, April 27 - April 29, 2013.
- Member of the Program Committee des Internationalen Workshops „Nanoscale pattern formation at surfaces", Kopenhagen, Dänemark, May 25-30, 2013.
- Member of the International Program Committee IVC-19 und des Steering Committee der Intl. Conference on Nanoscience + Technology (ICN+T 2013), Paris, Sept. 9 -13, 2013.

11. University Administration

Oskar Paris (MUL)
- Institutsvorstand (Chair): since 2009
- Vizestudiendekan (Vice Dean): since October 2011
- Senat Member: until 2013
- Curriculumskommission Werkstoffwissenschaften: Member
- Curriculumskommission Kunststofftechnik: Substitute Member
- Berufungskommission Materialphysik: Chair 2012
- Berufungskommission Materialphysik: Member 2013-2014
- Habilitationskommission Motz: Chair 2011/2012
- Habilitationskommission Oswald Tranta: Member 2013
- Habilitationskommission Bucher: Member 2013
- Habilitationskommission Kiener: Reviewer 2013
- Habilitationskommission Brunner: Reviewer & Member 2013

Ronald Meisels
- Curriculum Kommission „Doktoratsstudium"
- Habilitationskommission Brunner: Member 2013

Josef Oswald
- Institute of Physics: Vice Chair (until 7/2013)
- Senat (Vice Chair/ until 2013)
- Betriebsrat (Vize Chair/Chair/ Member)
- Universitätsgewerkschaft wissenschaftliches Personal, Bundesvertretung 13 der GÖD (Vice Chair)
- Verhandlungsteam der GÖD für den Universitätskollektivvertrag (Member)
- Habilitationskommission Brunner: Member 2013
- Mitglied des Satzungsarbeitskreises des Rektors (until 2013)
- Mitglied der Wahlkommission für die Senatswahl
- Mitglied der Wahlkommission für die Betriebsratswahl

Christian Teichert
- Institute of Physics: Vice Chair since 7/2013
- Curriculum Kommission „Werkstoffwissenschaften“ (Member)
- Berufungskommission Materialphysik 2012 (Member)
- Berufungskommission Materialphysik 2013-2014 (Member)
- Habilitationskommission Motz (Member): 2011/2012
- Habilitationskommission Zhang (Member): 2012/2013

12. Advisory- & Editorial Boards, Review Committes, Membership, etc.

Oskar Paris

Boards and Memberships

- Editorial Board Member of Scientific Reports, Nature Publishing Group (since 2012).
- Austrian Observer at the Council of the European Synchrotron Radiation Facility (ESRF) (since 2011).
- Chairman of the ESRF Advisory Board of the Austrian Academy of Sciences (since 2011).
- Member of the ILL Advisory Board of the Austrian Academy of Sciences (since 2012).
- Member of the Delegate Assembly of the Austrian Science Foundation (FWF).
- Chairman of the Neutrons and Synchrotron Radiation division (NESY) of the Austrian Physical Society (ÖPG) (since 2012).
- Member of the Metals and Materials division steering group of the German Physical Society (DPG) (since 2013).
- Member of the Austrian National Committee for Crystallography (OeNKK) (since 2013).
- Member of the Austrian Physical Society (ÖPG), German Physical Society (DPG), Materials Research Society (MRS), Friends of Helmholtz-Zentrum Berlin e.V., Austrian Chemical-Physical Society (CPG).

Review Committees

- Member of the German BMBF Gutachterausschuss „Erforschung kondensierter Materie an Großgeräten“: 2010-2013 and 2013-2016.
- Scientific Proposal Review Committee member at several large scale European Synchrotron and Neutron facilities: ESRF Grenoble (since 2012), FRM II, Munich (since 2010), Helmholtz-Center Berlin (2009-2012).
- Chairman of the Review committee of the EDDI-MAGS-SAXS, beamlines, Helmholtz-Zentrum Berlin (2012).
- Reviewer for several national science foundations (Germany, UK, Israel), and for a broad spectrum of scientific journals in Physics, Materials Science, Chemistry and Biology.

Ronald Meisels

- Member IEEE (Institute of Electrical and Electronic Engineers)
- Reviewer für European Physical Journal B, Optical, Applied Optics, Optical Engineering.
- Juror AYPT (Austrian Young Physisists Tournament).

Josef Oswald

- Gutachtertätigkeit BMWF/ÖAD
- Reviewer für Europhysics Letters, Physical Review B, Physical Review Letters
- Member of the Austrian Physical Society

Christian Teichert

- Austrian representative and since 2010 Secretary and since 2013 Chair of the Nanometer Structure Devision, IUVSTA
- Division Chair “Surfaces, Interfaces and Thin Films” Austrian Physical Society.

- Since 2013 Board Member, Austrian Physical Society.
- Referee for ÖAD, Czech, Polish and German Science Foundations, Netherland Organization of Scientific Research, Referee for Professorships (UCB, USA), Ph D Referee (TU Graz,)
- Member of the Austrian Physical Society (ÖPG), German Physical Society (DPG), Materials Research Society (MRS),American Vacuum Scociety (AVS), Austrian Vacuum Society (ÖVG).
- Juror AYPT (Austrian Young Physisists Tournament).

Markus Hartmann

- Juror AYPT (Austrian Young Physisists Tournament).

Markus Kratzer

- Betriebsrat (Member)
- Reviewer ACS Applied Materials & Interfaces, RSC Catalysis
- Juror AYPT (Austrian Young Physisists Tournament).

Rainer Lechner

- National Delegate for the European Synchrotron User Organisation (ESUO)
- Reviewer for Journal of Crystal Growth, Journal of Applied Crystallography, Journal of Applied Physics
- Juror AYPT (Austrian Young Physisists Tournament).

Picture Gallery

Nobelpreiskolloquium
13. December 2012, MU Leoben

Oskar Paris, Rector Wilfried Eichlseder, Helmuth Rauch (TU Wien), Klaus Richter (Uni Salzburg), Werner Sitte

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NESY-Symposium: Research at European Neutron and Synchrotron Facilities by Austrian Scientists", TU Wien, Nov. 11th/12th 2013

O. Paris (NESY Chairman)

Podium Discussion (from left): G. Bauer (Uni Linz), H. Abele (TU Wien), F. Uhlig (TU Graz), O. Paris (MU Loeben), J. Stangl (Uni Linz), Alfonso Franciosi (ELETTRA Trieste), J. Fröhlich (TU Wien), D. Weselka (BMWFW), H. Schober (ILL Grenoble), G. Krexner (Uni Wien)

17th International Winterschool on New Developments in Solid State Physics "Mauterndorf 2012, 12 - 17 Feb, 2012, Castle of Mauterndorf, A-5570 Mauterndorf, Province of Salzburg, Austria

Organizers of the International Winterschool "Mauterndorf 2012" with Nobel Prize laureate Klaus von Klitzing (from left: F. Schäffler, K. v. Klitzing, W. Jantsch, G. Bauer, F. Kuchar)

10. Werkstoffkongress, Next Generation of Materials and Devices from Bioinspiration, 6th/7th November 2013, Leoben, Austria

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Rigorosum Erko

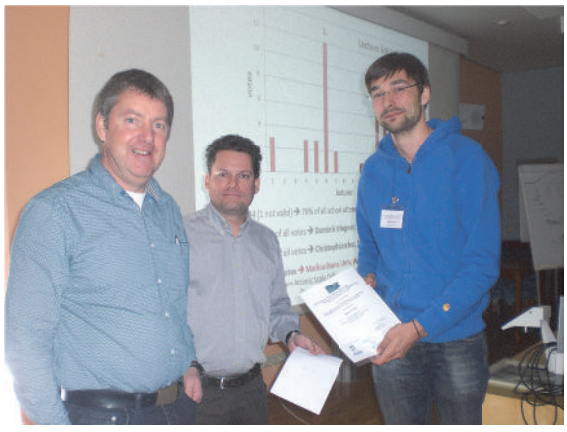
24 April 2012

Rigorosum Nevosad

5 December 2013

8th European NESY Winter-School & Symposium on Neutron- and Synchrotron Radiation, Planneralm (Austria), March 10-16, 2013

The “Young Scientist Best Poster Prize”: RiedRiedl Angelika, Materials Center Leoben For GmbH, Leoben



“Young Scientist Best Lecture Prize”: Stana Markus, Universität Wien, Fakultät für Physik / Dynamik kondensierter Systeme

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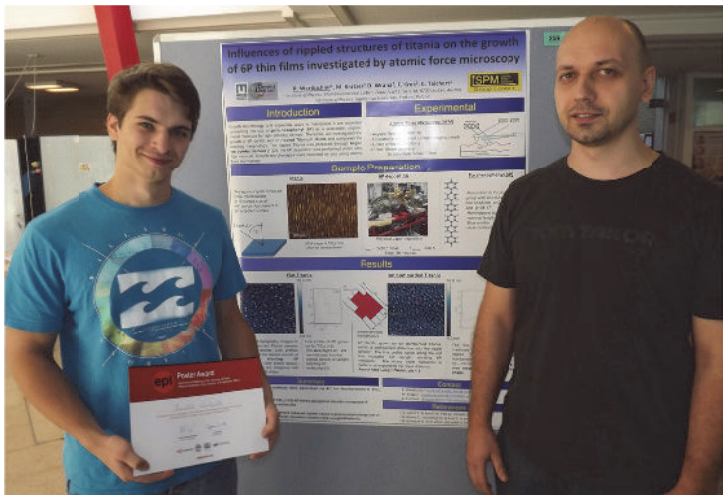
Excursion with Materials Science Students from Leoben to the synchrotron radiation source ELETTRA in Trieste, Italy. 19th/20th March 2012.

13. June 2012 in Stockholm, Presentation of the "Best Presenter Award" of the International Paper Physics Conference, Graz 2022 to Dr. Franz Schmied.

Ramin Farnood (University of Toronto, Canada), Warren Batchelor (Australian Pulp and Paper Research Institute, Monash University, Melbourne, Australia), Franz Schmied and Sören Östlund (KTH/Innventia, Schweden). (Foto: Johan Olsson)

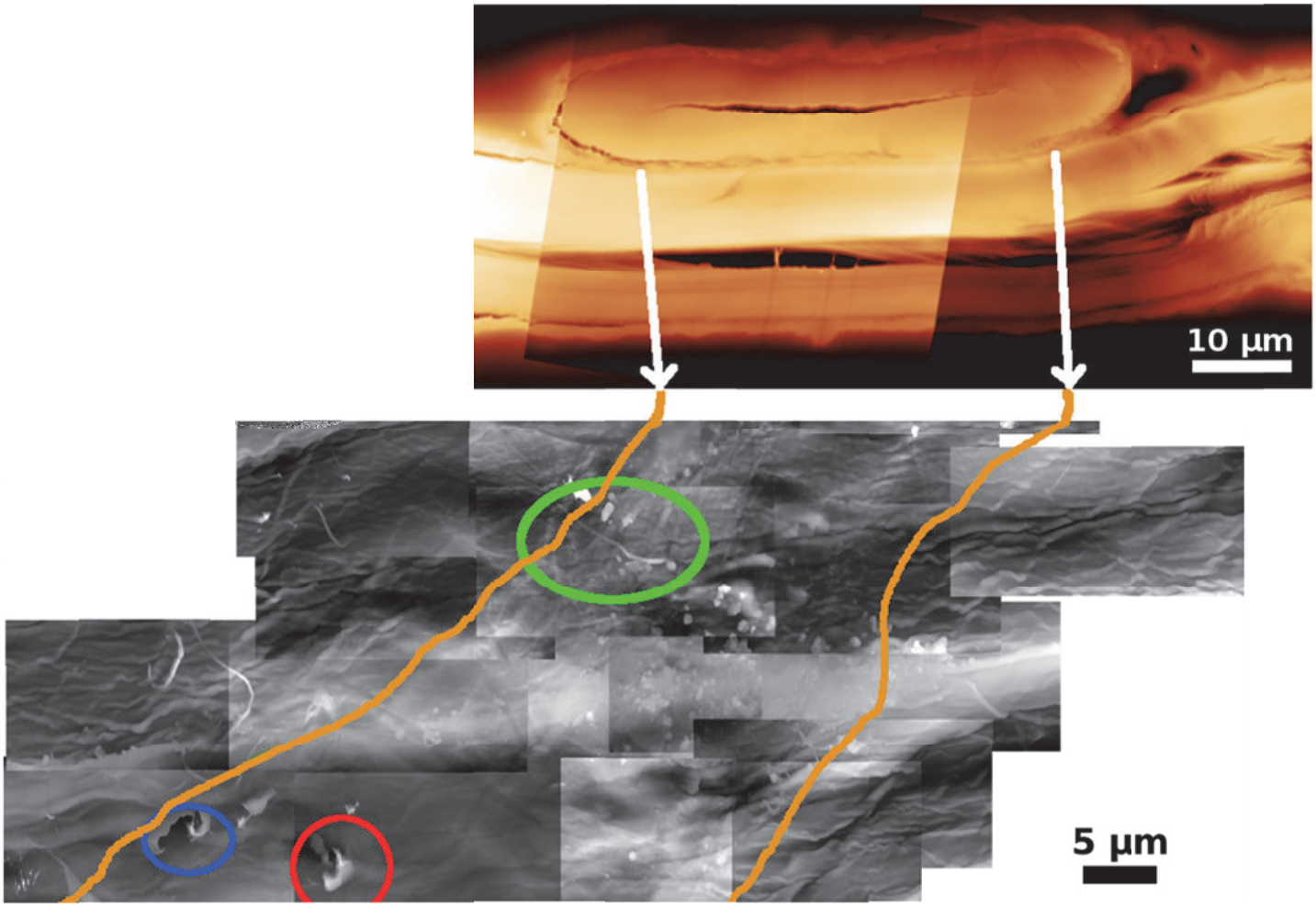
Poster Prize for Reinhold Wartbichler, Materials Science student in 6th semester for his poster presented at the Joint Annual Meeting of the Austrian and the Swiss Physical Society, Linz, 3.-6.9.2013.



Reinhold Wartbichler (with the certificate of the best poster) and Markus Kratzer at their poster at the Joint Annual Meeting of the Austrian and the Swiss Physical Society, Linz, 3.-6.9.2013.

Second Prize of the Best Physics Paper of Austrian High School students 2012 to Tomas Kamencek, who did experimental work in the Scanning Probe Microscopy Group of the institute.

Leopold Matelitsch (Graz), Gerhard Haas (Leoben), Thomas Kamencek and Christian Teichert at the Award presentation at the Austrian Physical Society meeting in Graz, Sept 2012.



Stitched AFM images of pulp fibers (Schmied et al. Nature Scientific Reports 2013)