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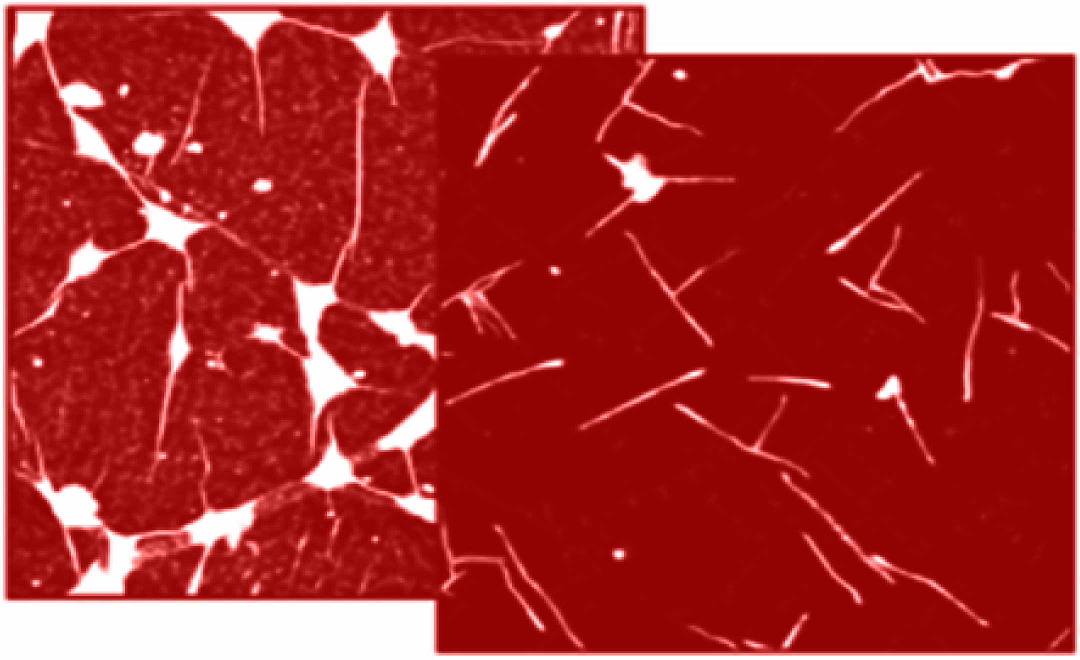
BI – ANNUAL REPORT
2014 and 2015



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Oskar Paris

Contact

Institute of Physics
Montanuniversität Leoben
Franz Josef Straße 18
A-8700 Leoben

Phone: +43 (0)3842 402-4601
Fax: +43 (0)3842 402-4602
e-mail: physics@unileoben.ac.at
http://www.unileoben.ac.at/physics

Cover picture: AFM images of organic thin film growth on graphene substrate

Institut für Physik

Montanuniversität Leoben

BI-ANNUAL REPORT

2014/2015

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Preface

Dear colleagues and friends,

It is a pleasure to present this bi-annual report, providing a comprehensive overview of the research- and teaching activities of the Institute of Physics at the Montanuniversität Leoben in the reporting period 2014 and 2015. Some exciting new scientific activities, several new co-workers, and many new students: this is what makes life at our institute interesting, diversified, but also challenging. Our scientific mission to conduct high-level basic research related to “Physics of Functional Materials for Electronics, Photonics and Energy” goes hand in hand with research-guided teaching in “Materials for Electronics and Physics of Functional Materials” for materials science Master students. Besides this, the basic physics education of all Bachelor students at the Montanuniversität Leoben continues to keep us busy, given the considerable increase of freshmen students particularly within the last two years.

The core of this report constitutes 15 short research reports on scientific projects, most of them being related to doctoral- and/or master theses that are/were conducted at the institute. The publication output from these activities in the reporting period amounts to 60 publications, the vast majority of them (55) beeing peer-reviewed papers in SCI listed journals. Several papers were published in high-impact journals, for instance in *Energy and Environmental Science* (IF 25.4), *ACS Nano* (IF 13.3), *Advanced Functional Materials* (IF 11.8), or *Physical Review Letters* (IF 7.6). I am particularly delighted that some of this work has been explicitly highlighted by the journals or by other print media, or has found its way to the cover pages of the respective issues. Almost 100 high-level presentations were given at national and international conferences, and members of the institute have organized or co-organized conferences and schools themselves. Several members of the institute have received awards or honors for their work, all this being listed together with many other achievements at the end of this report.

The acquisition of research funds becomes 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 almost one Million Euro were executed during the reporting period. I am particularly enthusiastic that several international and interdisciplinary projects could be started during the reporting period: A joint Austrian-German- and a joint Austrian-French project within the international-program line of the Austrian Science Foundation (FWF), a COMET-K2 project with an international company partner, a national cooperation project funded by the Austrian “Klima- & Energiefonds”, and the participation in a CD-Laboratory. Not to forget are several smaller projects (e.g. ÖAD) and a total of 60 days of beamtime at large scale facilities for synchrotron- and neutron radiation. Finally, we could also expand our Lab research infrastructure towards two new instruments for small-angle X-ray scattering (SAXS), and we have developed new in-situ equipment in combination with SAXS related to gas-adsorption and to electrochemistry, respectively.

Since I started working at the Institute of Physics in 2009, the personnel situation is more or less unchanged at around 20 staff members. Roughly half of the scientific staff is being financed from third party money. This has to be seen in the context of the continuously increasing number of freshmen students, which continues to shift the major duties of the faculty staff towards teaching at the expense of research. For instance, two former young research assistants are now assigned senior lecturers with a much higher teaching duty than before. I also notice a very strong increase of the number of teaching classes and essentially a doubling of the total number of exams since 2009. Although it will definitely not become easier to keep a sane balance between teaching and research in the future, I see it as my major responsibility to facilitate both, high-quality education and cutting-edge research, and to enable scientific career opportunities to young academics beyond pure knowledge teaching. The habilitation of Roland Brunner (more habilitations to come soon), the appointment of a half-year guest professorship to Gerhard Popovski, or the celebration of “30 Jahre Werkstoffe der Elektronik” during the reporting period may serve as examples that this works in the long term.

Our progress and achievements would not have been possible without motivated coworkers and numerous cooperation partners. I am 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.

August 2016 Univ.-Prof. Dr. Oskar Paris

1. Personnel

Faculty: Science and Teaching

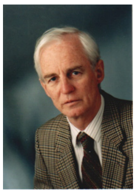
Professors

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

Ao.Univ.-Prof. Dr. Christian TEICHERT
(Vice-Chair)

Ao.Univ.-Prof. Dr. Josef OSWALD

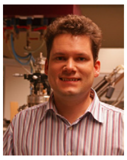
Ao.Univ.-Prof. Dr. Ronald MEISELS



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

Assistants

Dr. Markus HARTMANN
Assistant/Senior Researcher
(until 04/2015)



Dr. Rainer LECHNER
Assistant/Senior Lecturer

Dr. Markus KRATZER
Assistant/Senior Lecturer

Dipl.Ing. Roland MORAK
Assistant/PhD Student

Dipl.Ing. Christian KOCZWARA
Assistant/PhD Student (since 9/2015)

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Heide KIRCHBERGER
(Secretary)

Magdalena OTTRIN
(Secretary)
(until 01/2015)

Thomas JUD
(Apprentice to the Secretariat)
(since 09/2015)

Peter MOHARITSCH
(Mechanical Engineer)

Ing. Heinz PIRKER
(Electrical Engineer)

Research Associates and Students workers

Postdocs

Dr. Parvin SHARIFI
Postdoc (until 5/2014)

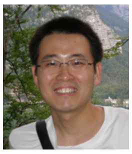
Dr. Gerhard POPOVSKI
Postdoc

PhD students

Dipl.Ing. Christian GANSER
Doctoral student
(unitil 5/2015)

Dipl.Ing. Christian PREHAL
Diploma thesis (until 3/2014)
Doctoral student (since 04/2014)

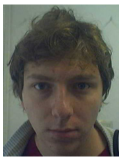
MSc Benjamin Kaufmann
(since 2/2015)



Dipl.Ing. Quan SHEN

MSc. Seyedsoran NABAVI
(until 4/2015)

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



Dipl.Ing. Lukas Ludescher
Diploma thesis (until 2/2016)
Doctoral student (since 3/2016)

Diploma thesis

Max BURIAN
Diploma thesis (until 6/2014)

Patrice KREIML
Student Worker,
Diploma thesis (until 6/2016)

Catherina CZIBULA
Student Worker,
Diploma thesis

Jakob Alexander GENSER
Student Worker,
Diploma thesis (since 10/2015)

Stefan KLIMA
Diploma thesis (until 6/2015)

Michael HUSZAR
Diploma thesis (since 6/2015)

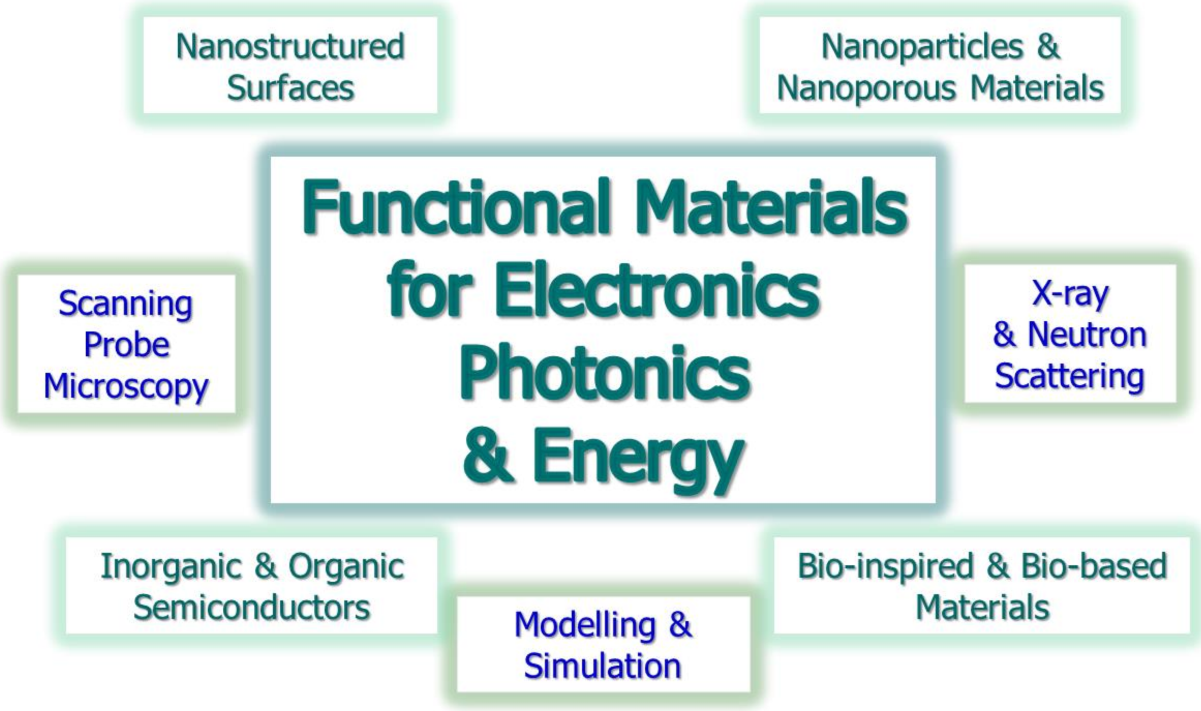
Student Workers

Michael LASNIK
Student Worker,

Hannah SCHÖNMAIER
Student Worker

2. Research

Research at the Institute of Physics is dedicated mostly to the physics of functional materials. Actual research topics include the study of nanostructured surfaces, nanoparticles and nanoporous materials, as well as biological, bio-inspired and bio-based systems. In particular we investigate the (nano-) structure and functional properties of a wide range of materials such as graphene, semiconductor nanoparticles, ordered nanoporous silica and -carbons, or paper fibers. Potential application fields are in electronics (including electronic transport phenomena), photonics, and energy conversion (solar cells) and storage (supercapacitors and batteries).Two major experimental methods are employed namely scanning probe microscopy and scattering techniques, including the extensive use of synchrotron- and neutron radiation at large-scale facilities. Experimental work is complemented by a range of numerical simulation tools such as atomistic Monte Carlo simulations, finite difference time domain (FDTD) calculations, or quantum mechanical simulations.



Currently the 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, Markus A. Hartmann, Christian Koczwara, Rainer T. Lechner, Lukas Ludescher, Soran Nabavi, Roland Morak, Gerhard Popovski, Christian Prehal, Hannah Schönmaier, Parvin Sharifi

Surface Physics and Scanning Probe Microscopy: ***Christian Teichert***
Catherina Czibulka, Christian Ganser, Jakob Genser, Michael Huszar, Benjamin Kaufmann, Stefan Klima, Markus Kratzer, Patrice Kreiml, Michael Lasnik, Monika Mirkowska, Quan Shen

Photonics and Nanoelectronics: ***Ronald Meisels***
Friedemar Kuchar

Simulation Electric Transport: ***Josef Oswald***

The following pages compile the research reports from these groups in the reporting period 2014/2015.

Nanomaterials & Scattering

Functional Nanoparticles

Rainer T. Lechner, Max Burian, Lukas Ludescher, Gerhard Fritz-Popovski, Oskar Paris
rainer.lechner@unileoben.ac.at

1) Core/shell structure and shape of nanocrystals influences their optical properties

The wet chemical synthesis of core/shell colloidal nanocrystals (NCs) has led to a pronounced improvement in the optical properties and the chemical stability of semiconducting NCs [1, 2].

The infrared emission of lead chalcogenide nanocrystals (NCs) can be drastically increased by stabilising the core with a hard protective shell [1]. For the cationic exchange based shell growth of PbS/CdS NCs [3], we have shown that metastable crystal phases in the chemical homogenous CdS shell influences significantly the photoluminescence (PL) emission.

We could show that the chemical uniform CdS shell keeps the cubic *rock salt* (*RS*) structure of the PbS core in the early stages of transformation, and takes only after some time the equilibrium *zinc blende* (*ZB*) structure of CdS (see Fig. 1a). Furthermore, the *RS*→*ZB* phase transition mechanisms depend on the thickness of the CdS shell. This could be only reveald by retrieving the chemical profile of NCs in sub-nanometer resolution by using anomalous small angle x-ray scattering (ASAXS) in combination with the analysis of powder diffraction data retrieved by wide angle x-ray scattering (WAXS). The metastable *RS* phase fraction within the shell, however, directly influences the PL output, whereas the PL enhancement is most suppressed for CdS shells exceeding 1nm thickness (see Fig. 1b).

In a recent study performed at the European synchrotron radiation facility (ESRF), we have investigated also CdSe/CdS core/shell NCs with different dimensions by recording simultaneously ASAXS and WAXS spectra. In contrast to the CdS shells around PbS cores [3], here the CdS shells were grown *epitaxial* on nominal spherical CdSe cores in hexagonal *wurtzite* structure [2].

We revealed that the epitaxial core/shell structure depicts the same sharp chemical interface as found for the PbS/CdS system, even after a post growth annealing step. With increasing NC diameter, however, the CdSe/CdS NCs deviate significantly from a spherical shape. By means of a recently developed shape retrieval method for SAXS data of colloidal NCs [4], we could reveal an elliptical particle shape with pronounced surface facets for the largest core/shell series (see Fig. 1c). By comparing the Bragg peak widths of the recorded powder diffraction pattern with the NC dimensions derived from SAXS we could relate the short axis to the tilted (101), (102) and (103) crystal planes, whereas the long axes are formed by the straight (100), (110) and (001) planes. We could also directly relate the core/shell structure and the NC shape to the PL performance, i.e., the elliptical and faceted CdSe/CdS NCs depicts the lowest PL quantum yield.

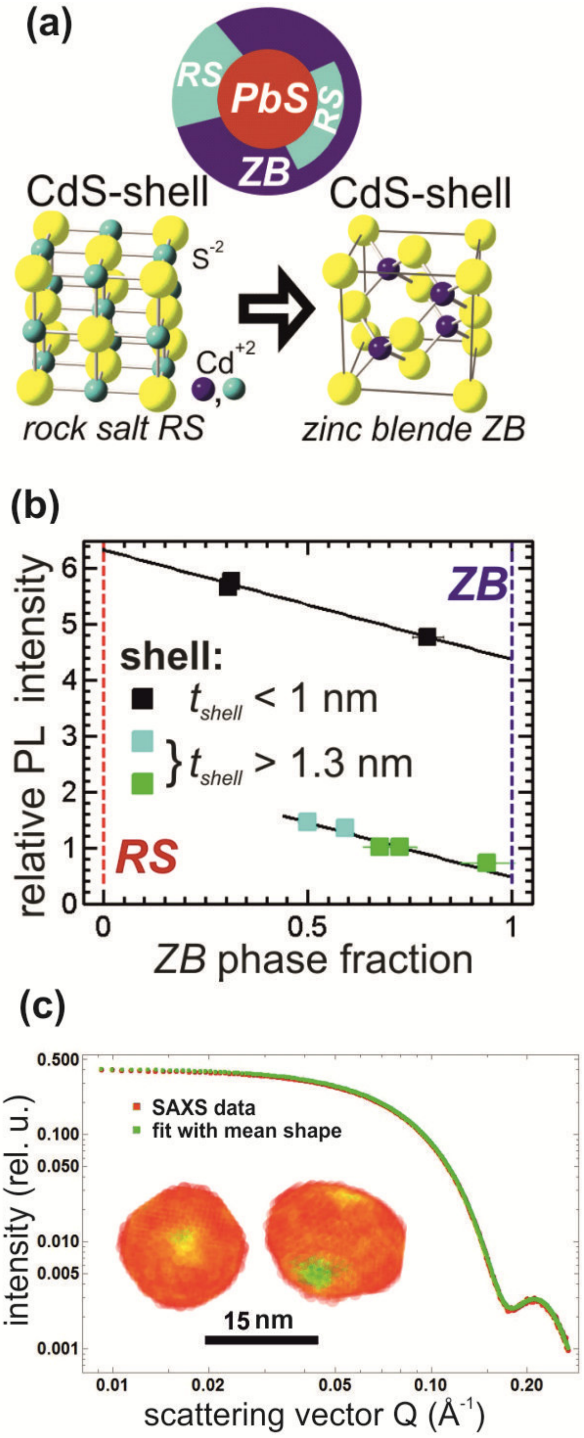


***Figure 1:* (a)** *Metastable crystal phases in the CdS shell of PbS/CdS core/shell NCs derived combining ASAXS and WAXS.* **(b)** *Influence of the crystal phase fractions within the shell on the PL emission* **(c)** *From SAXS data derived elliptical and faceted mean shape of CdSe/CdS core /shell NCs.*

2) Nanocrystal shape impacts the lasing threshold in partly ordered nanocrystal films The shape of CdSe/CdS NCs not only influences the PL output of individual NCs, but has also a major impact on the lasing properties of a partly ordered NC-film on a substrate [5]. With grazing incidence SAXS (GISAXS) we revealed the mean separation and the degree of ordering of different

CdSe/CdS NC aggregates. The NCs are separated by organic ligands and hence the amount of the inorganic NCs volume fraction is the key feature for optimised random lasing. Indeed, we could show with our analysis of the GISAXS scattering patterns that the non-spherical CdSe/CdS NCs exhibit the lowest NC volume fraction and thus show the highest laser threshold.

To conclude, the morphological properties and the volume fractions of the NCs in the films, which have been mainly obtained by GISAXS, turned out to be more important to achieve low lasing thresholds as the quantum yield of the individual NCs [5].

3) Structure and shape of nanocrystals impact the supercrystal structure of colloidal superlattices

The mean shape of NCs can also significantly influence the supercrystal structure of well-ordered colloidal superlattices [1], where the individual NCs are used as building blocks. We have shown this by investigating the self-assembly of colloidal supercrystals based on nearly monodisperse Bi NCs with *in-situ* synchrotron SAXS at the Austrian SAXS beamline at the synchrotron radiation source ELETTRA [6]. We studied the colloidal crystallization by diffusion of a non-solvent into the colloidal dispersion of Bi NCs [7]. The SAXS patterns of the NC ensembles were recorded below the NC-solvent/non-solvent interface (see Fig. 2a). Hence, we could follow the onset of the crystallization process in short time steps as a function of the non-solvent concentration.

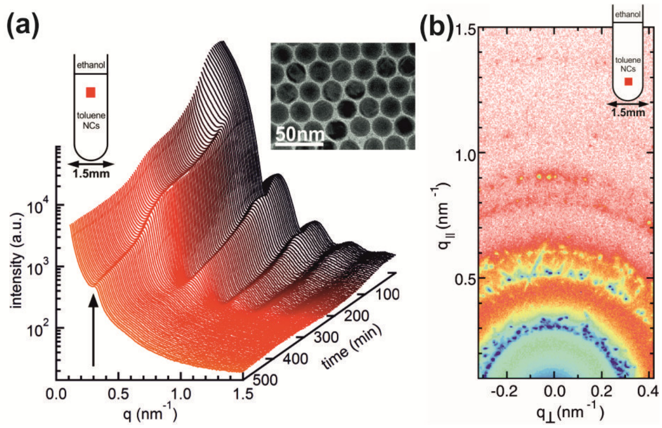


Figure 2: (a) *In-situ 1D SAXS patterns plotted over the length of the scattering vector q and time during self-assembly of colloidal supercrystals using Bi-NCs (see TEM inset) as building blocks. The beam was positioned few millimeters below the non-solvent/solvent interface.* ***b)*** *2D diffraction pattern from many micrometer sized individual supercrysrals. The 2D SAXS patterns were recorded several millimeters away from the interface.*

Further away from the solvent/non-solvent interface the supercrystal growth is slowed down, resulting in well-ordered 3D colloidal supercrystals with ordered domain sizes in the micrometer range. This is deduced from the analysis of the very sharp individual superlattice peaks visible in the 2D reciprocal space map shown in Fig. 2(b). To test, if the experimentally obtained supercrystal structure is related to the equilibrium superstructure of densely packed Bi-NCs, our colleagues from the Computational Physics Group of the University of Vienna theoretically model the crystallization process based on Monte Carlo simulations [7].

As an input for these simulations, we need the exact 3D shape of the individual Bi Ncs. For obtaining this shape we developed a new method to retrieve the *mean* particle shape of a large ensemble (~ 10^8 NCs) of slightly polydisperse nanoparticles by advanced SAXS analysis methods [4]. The resulting shape deviates significantly from a sphere and can be described by a strongly facetted oblate ellipsoid related to the *rhombohedral* crystal structure of Bi. The largest surface facet is formed by the (001) crystal plane, whereas also the shortest axis of the NC is along the *rhombohedral* c-axis.

The resultant mean shape was used for the theoretical modelling of the crystallisation process. Thus we can directly compare simulated and experimental derived diffraction patterns. Simulations and experiments show a good agreement and hence we are able to link the supercrystal structure via the NC-shape to the atomic Bi crystal structure.

Cooperation

- W. Heiss, M. Sytnyk (JKU Linz & FAU Erlangen-Nürnerg)
- M. Kovalenko (ETH Zürich & EMPA Dübendorf)
- M. Yarema (ETH Zürich)
- A. Hoell (HZB-BESSY II, Berlin)
- T. Narayanan, T.U. Schülli (ESRF, Grenoble)
- H. Amenitsch (TU Graz & ELETTRA, Triest)
- C. Karner, C. Dellago (Univ. Wien)

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[7] M. Yarema, et al., ACS Nano 6, 4113 (2012)

Nanomaterials & Scattering

Electrosorption in Microporous Carbons

Christian Prehal, Christian Koczwara, Hannah Schönmaier, Oskar Paris
christian.prehal@unileoben.ac.at
oskar.paris@unileoben.ac.at

In the last two years we have introduced a new method of *in-situ* small-angle x-ray scattering (SAXS) applied to nanoporous carbon based supercapacitors during charging and discharging. We have developed special in-situ devices consisting of two stacked carbon electrodes separated by a separator and covered by current collectors. Small holes in all layers except the working electrode allows following the change of the SAXS signal and the x-ray transmission signal as a function of a variable voltage signal applied to the device via a potentiostat. Time resolved experiments were conducted at the Austrian SAXS beamline at the synchrotron radiation source ELETTRA in Trieste. X-ray transmission experiments and slow cycling SAXS experiments are also feasible with the laboratory SAXS instruments available.

1) Local and global ion rearrangment

Efficient and fast storage of electrical energy is essential for a sustainable energy management based on green technologies like, wind or solar energy conversion, or electric cars. Supercapacitors reveal high power density, good efficiency, and ultra-long cycle lifetime. If a pair of nanoporous carbon electrodes is immersed into an electrolyte reservoir, an electrical double-layer is formed at the electrode-electrolyte interface as soon as a voltage is applied. Energy is stored via ion electrosorption, where the opposite charge of electrons/holes on the electrode side and anions/cations on the electrolyte side reveal the capacitive behavior. Traditionally the charge storage was explained by ions being adsorbed on both pore walls within slit like pores. Severe confinement issues arise when we consider that the pore size in nanoporous carbons is around the size of the ions themselves. The exact understanding of ion re-arrangement in the charged confinement of carbon nanopores is essential for improving the performance of supercapacitor- and related technologies like, e.g., capacitive deionization (CDI) used for water treatment.

With conventional electrochemical methods, only limited information on molecular details of ion electrosorption phenomena can be obtained. Hence, novel experimental approaches are urgently needed which are able to probe local ion arrangement as a function of an applied voltage. We employed time-resolved SAXS to study the working electrode of model supercapacitor cells using a commercially available activated carbon with an average pore size of 1.3 nm, and three different aqueous solutions at 1 M concentration (CsCl, KCl, NaCl) as electrolytes. While we applied various time dependent voltage signals, the SAXS patterns and the corresponding x-ray transmission values are recorded. The transmitted intensity of the primary beam depends on the cation and anion concentration within the working electrode weighted by their x-ray absorption coefficients. Therefore, the x-ray transmission together with the independently determined electrical current allows the calculation of cation and anion concentrations independently from each other. The results demonstrate that for all electrolytes the electrode charge is counterbalanced via pure ion swapping, that is, for each counter-ion entering the pores, exactly one co-ion is expelled from the pores, with the total ion concentration within the electrode remaining constant (see Fig. 2a).

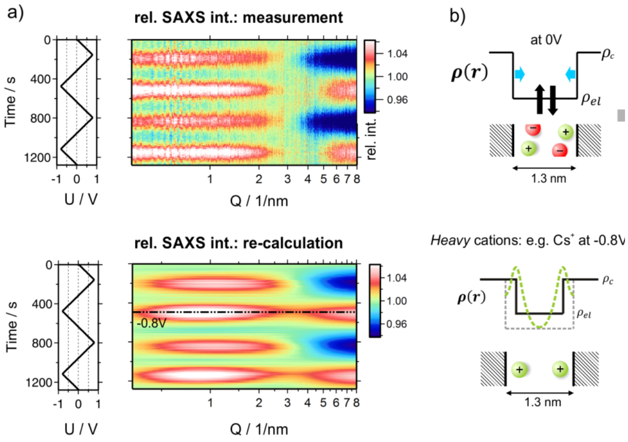

Figure 1: *a) (top): relative SAXS intensity as a function of time and length of the scattering vector length Q for a 1M aqueous CsCl electrolyte during voltage cycling. The re-calculated data (a), bottom) were obtained by considering a simple two-phase model picture as sketched in b).*

In Fig. 1a (top) the relative SAXS intensity as a function of time (or applied voltage) and the scattering vector length Q is shown. A simple, yet effective way to understand the rather complex change of the SAXS intensity is to calculate the radius of gyration R_g (Fig. 2b). The magnitude of R_g was found to closely correlate with the counter ion electron number (Fig. 1b). Within a simple two-phase model the change of the SAXS intensity can be described consistently by a changing electron density difference together with an apparent change of the pore width due to the preferred adsorption of counter-ions close to the pore walls (see sketch of electron density profiles in Fig. 1b). Using the well-known Debye-Anderson-Brumberger (DAB) model to analytically back-calculate the SAXS intensity changes, excellent agreement with the measured data is found (Fig. 1a top vs. bottom). The quantitative back-calculation however only works when considering a densified hydration shell depending on the specific ion (Na^+, K^+, Cs^+, Cl^-). This underlines the importance of the explicit role of water during ion electrosorption. Considering the combined results from SAXS and x-ray transmission, a comparison of the ion transport on a *local* vs. the *global* scale is possible (comparing Fig. 2a and Fig. 2b).

While the actual electrosorption is accommodated by ion swapping involving both, co-ion expulsion and counter-ion adsorption, *locally* only counter-ions move preferably from the center towards the pore walls as a voltage is applied.

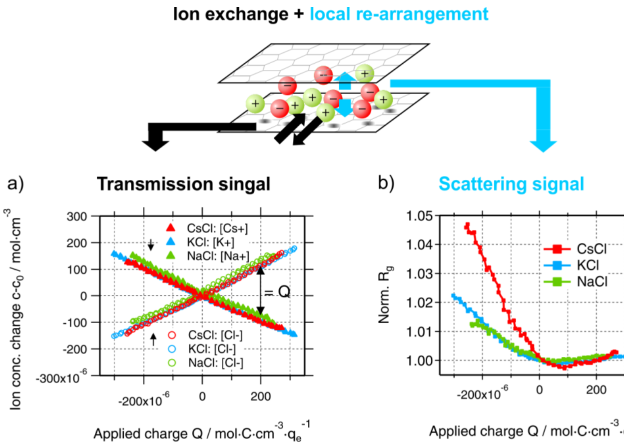

***Figure 2**: a) Cation and anion concentration as a function of the applied charge, obtained from x-ray transmission measurements. In b) the relative change of the radius of gyration from SAXS as a function of the applied charge is plotted..*

2) Gaussian random fields – a novel way to produce 3D real-space pore structures

For the *in-situ* study of time-dependent processes like ion electrosorption in porous materials, realistic real-space models of pore structures are desirable. Having a real-space porous carbon structure, the pores can be "filled" with molecular species like ions or water molecules. Arranging them properly and weighting the real-space structure with the corresponding electron densities allows the re-calculation of a scattering curve using a simple discrete Fourier transformation. Such an approach may be of great relevance, since the calculated scattering curves can be directly compared with measured in-situ SAXS data, allowing different electrosorption models to be validated.

We have started to describe the structure of nanoporous carbons using 3D gaussian random field (GRF) defined as followed:

$$y(\boldsymbol{x}) = \sqrt{\frac{2}{N}}\sum_{i=1}^{N}\cos(\boldsymbol{k_i}\cdot\boldsymbol{x}-\varphi_i),$$

where the *k*-vectors have a length according to the distribution shown in Fig. 3b and a random direction. The shape of this distribution contains the information about size and morphology of the pore structure and can be derived from the measured SAXS pattern of the porous system. The phase shift φ_i is randomly distributed betwenn 0 and 2pi. A cross section of the resulting 3D GRF is shown in Fig. 3a, where the values *y(**x**)* are gaussian distributed according to Fig. 3c. Depending on the pore volume fraction a threshold value can be defined. All regions in *y(x)* above this value correspond to the carbon phase, all other values to the pores. This leads to the 3D real space pore structure shown in Fig. 3d.

Funding

- Austrian competence center program COMET K2 MPPE, Project A2.19.
- Austrian "Klima- und Energiefonds" under the program line "Energieforschung", Project 848808.

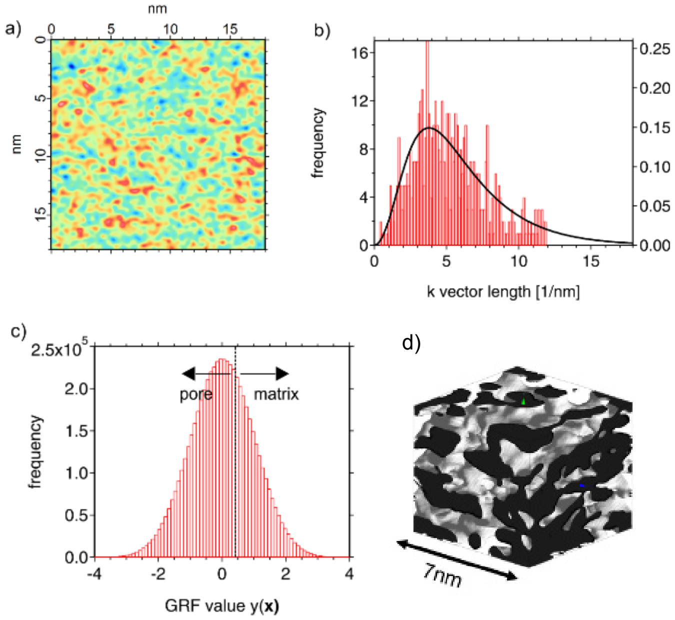

***Figure 3:** a) Cross section of the 3D Gaussian random field (GRF) y(**x**). b) k-vector frequency distribution, which is needed for the calculation of the GRFs. c) a histogram of all y(**x**) values is given. d) a 3D GRF derived pore structure is shown.*

Cooperation

- Volker Presser, Institut für Neue Materialien (INM) Saarbrücken.
- Nicola Hüsing, Univ. Salzburg.
- Heinz Amenitsch, TU Graz and ELETTRA Trieste.

References

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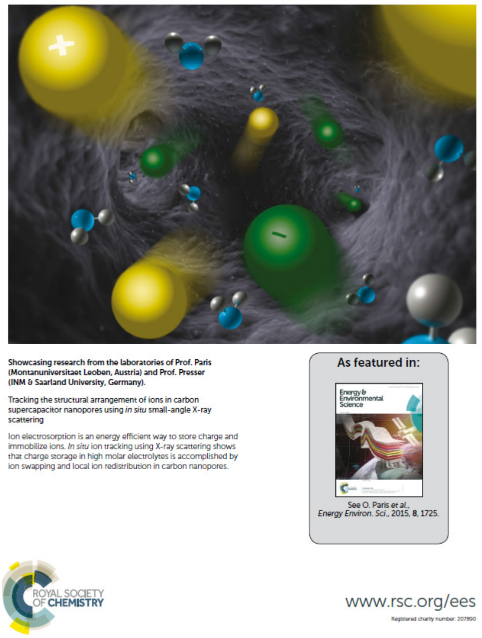

Showcasing research from the laboratories of Prof. Paris (Montanuniversitaet Leoben, Austria) and Prof. Presser (INM & Saarland University, Germany).

Tracking the structural arrangement of ions in carbon supercapacitor nanopores using *in situ* small-angle X-ray scattering

Ion electrosorption is an energy efficient way to store charge and immobilize ions. *In situ* ion tracking using X-ray scattering shows that charge storage in high molar electrolytes is accomplished by ion swapping and local ion redistribution in carbon nanopores.

As featured in:

Energy & Environmental Science

See O. Paris *et al.*, *Energy Environ. Sci.*, 2015, 8, 1725.

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The authors were invited to design the back-cover art of the corresponding issue of Energy Environ. Sci.

Nanomaterials & Scattering

Fluid Sorption in Mesoporous Silica

Roland Morak, Gerhard Fritz-Popovski, Lukas Ludescher, Oskar Paris
roland.morak@unileoben.ac.at
gerhard.popovski@unileoben.ac.at
oskar.paris@unileoben.ac.at

1) Sorption induced deformation of silica monoliths with hierarchical porosity

Sorption-induced deformation of nanoporous materials is of considerable interest in science and technology. Especially monolithic samples consisting of several hierarchies of pores with well defined pore sizes [1] are interesting objects in this respect due to their potential applications as sensors or actuators. We have investigated hierarchically organized porous silica monoliths consisting of a macroporous network of struts, each strut containing well-defined cylindrical mesopores of about 8 nm arranged on a 2D hexagonal pore lattice.

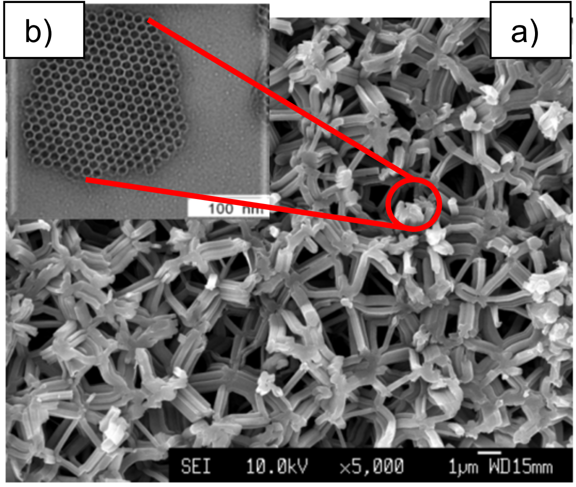

Figure 1 *a) Scanning electron microscopy (SEM) image of a monolithic silica sample. b) Transmission electron microscopy (TEM) image of a single strut with hexagonal order of mesopores (Courtesy N. Hüsing, Univ. of Salzburg).*

The deformation of this material induced by the sorption of n-pentane at the level of the mesopores has been studied with in-situ Small-angle X-ray scattering (SAXS). Due to the high 2D order of the pore lattice, the sorption induced strains in the radial direction of the pores can simply be obtained from the shift of the Bragg reflections. In addition, deformation on the macroscopic level was monitored with in-situ dilatometry [2]. The results (Fig. 2) show that the strains obtained by both methods have a qualitatively similar dependence on fluid pressure, but differ quantitatively. The general shape of these strain isotherms follow the three steps of the volumetric sorption isotherm [3]. These steps are the mono- and multilayer formation in the lower pressure regions (from point D to C) where an expansion of the material is observed due to the so called "Bangham effect" caused mainly by the change of the solid-liquid interfacial energy [3]. In the middle section (C-B) the pores are rapidly filling with the sorbent. Capillary condensation leads to a maximum negative Laplace pressure due to the hemispherical meniscus separating the liquid phase in the pores and the vapour phase outside. This leads to rapid pore contraction seen in Fig 2. The increase of the curvature radius of the meniscus with further increasing vapour pressure (B-A) continuously lowers the Laplace pressure, leading again to an expansion.

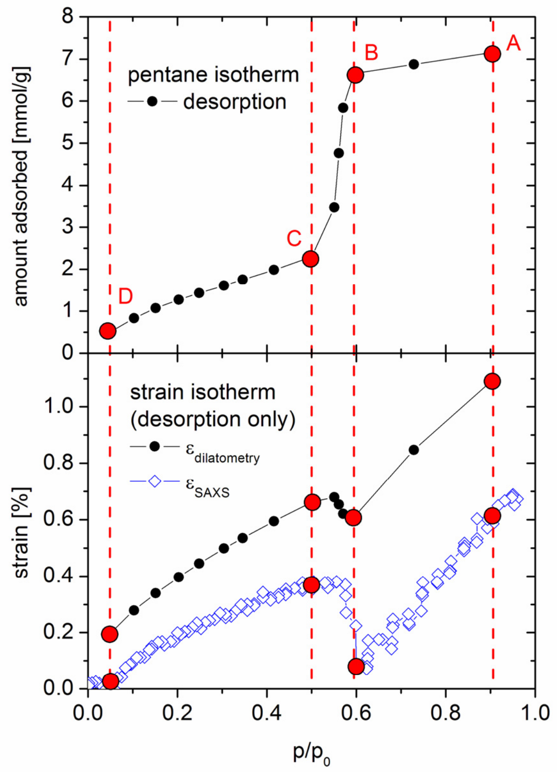

Figure 2 *Comparison of volumetric sorption isotherm (upper figure) and strain isotherms (lower figures) obtained by in-situ dilatometry and in-situ SAXS*

These results are very interesting for potential applications in the field of actuators. In order to control the sorption induced deformation at different levels of hierarchy, our cooperation partner (N. Hüsing, Univ. Salzburg) has developed a new synthesis strategy which allows influencing the orientation of the mesoporous struts leading to a macroscopically anisotropic network. The mesoporous struts being preferentially oriented parallel to the axis of the cylindrically shaped macroscopic monoliths make a sorption induced directional movement for actuation purposes in principle feasible.

Still, data analysis is a challenge due to the fact that the strains are rather small. To separate scattering contrast effects due to adsorbate uptake from real strains, in-situ small-angle neutron scattering (SANS) with "zero scattering-length water" was combined with in-situ dilatometry to investigate the pure mechanical response on two hierarchical levels simultaneously. These experiments - being currently still under evaluation - will help to understand the most important structural elements for the sorption induced deformation of hierarchical porous materials and how to control/taylor the structure for actuation applications.

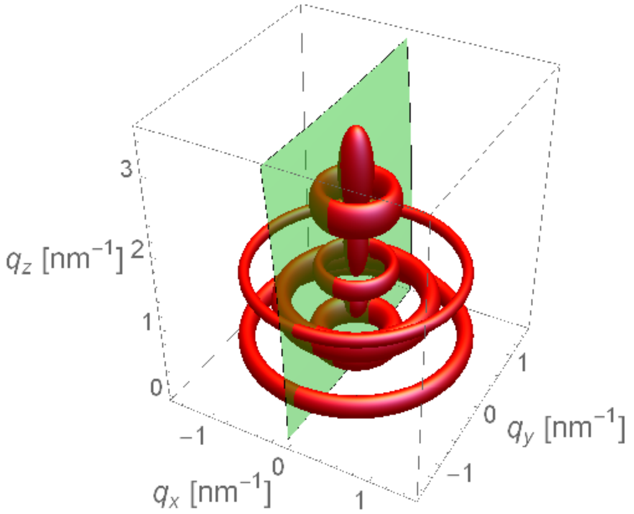

***Figure 3**: The peaks observed for a mesoporous film in reciprocal space. The cut created by the Ewald sphere is indicated in green.*

2) Mesoporous films

Evaporation induced self-assembly is a common technique to template ordered mesoporous films on surfaces. By this method, mesoporous materials with ordered cylindrical pores on a 2D lattice with the cylinder axis lying preferentially within the film plane can be synthesized via spin-coating or dip-coating. The final step of film preparation is calcination, i.e. the removal of the organic template by heating the structure to 500-600 °C in air. This step is accompanied by strong volumetric shrinkage of the nanostructure. The presence of the substrate prevents the material to shrink laterally, and therefore only the film thickness is reduced. This leads to a distortion of the originally hexagonal pore lattice and, as one might suspect, also of the original circular pore cross section.

The high order of the pores leads to pronounced Bragg peaks in the scattering pattern measured in reflection at small angles under grazing incidence geometry (GISAXS). Taking into account that the measured scattering pattern is only a cut of the Ewald sphere trough the reciprocal space and that the lack of preferential orientation of the pore axes within the film plane induces a cylindrical symmetry around the surface normal, one can reconstruct the complete reciprocal space (Fig. 3). Integration of the intensity of individual peaks over the whole reciprocal space results in integrated intensity values containing only form factor contributions. This information can be used to approximate a model for the cross section of the pores (Fig.4) [4]. The length ratio of the short to the long axis of the elliptical pore cross-section was found to be in the range from 0.44 to 0.57, slightly depending on the shear rate during preparation. This compares well with the deformation of the lattice as can be directly deduced from the positions of the Bragg peaks (Fig. 4a). The originally hexagonal lattice is deformed to an almost quadratic centred lattice by preferred vertical shrinkage of the unit cell. The resulting height of the new unit cell was found to be about 0.5 to 0.6 of the height found for the original hexagonal one [5].

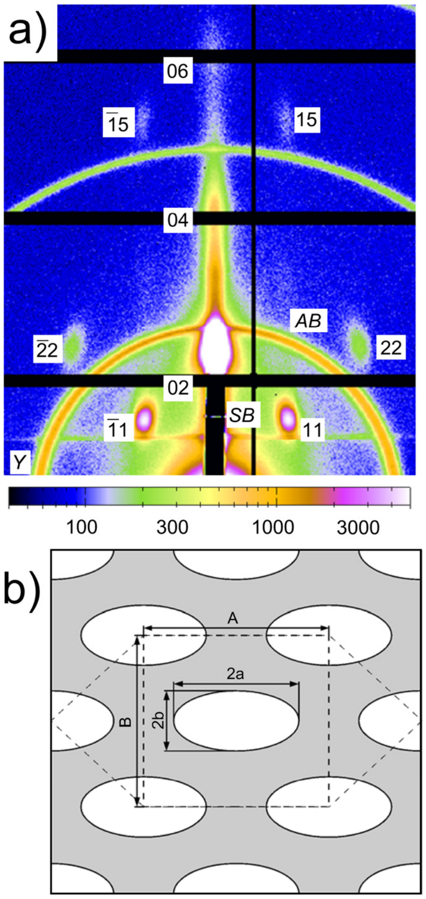

***Figure 4**: a) GISAXS pattern; b) Real space pore lattice with elliptical pore cross-section*

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Cooperation

- Gudrun Reichenauer (ZAE Bayern, Würzburg, D).
- Nicola Hüsing (Univ. Salzburg).
- Alex Neimark (Rutgers University)
- Gennadi Gor (Princeton University)
- Heinz Amenitsch (TU Graz)

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Nanomaterials & Scattering

Further Development of Scattering Techniques

Gerhard Fritz-Popovski, Roland Morak, Christian Prehal, Oskar Paris
gerhard.popovski@unileoben.ac.at
roland.morak@unileoben.ac.at
christian.prehal@unileoben.ac.at
oskar.paris@unileoben.ac.at

1) In-situ small angle X-ray scattering during fluid adsorption and desorption

The investigation of porous materials and their interaction with fluids during sorption is a subject of interest to many fields in research and industry (see previous reports).

The in depth study of such systems requires to study structural changes at the nanometer scale during fluid uptake and release. We have used SAXS as an analytical tool in this respect, and have developed in-situ sorption systems to be employed mainly at synchrotron radiation beamlines. Within a Project funded by Austrian Competence Center Programme COMET we currently develop an in-situ sorption system for a commercial Lab SAXS instrument (Bruker N8 Horizon). The system specifications will allow to determine volumetric sorption isotherms for various fluids in a temperature range from 50K to 350K and a preessure range from 0.1mbar – 1bar, where for each pressure step a SAXS pattern is recorded.

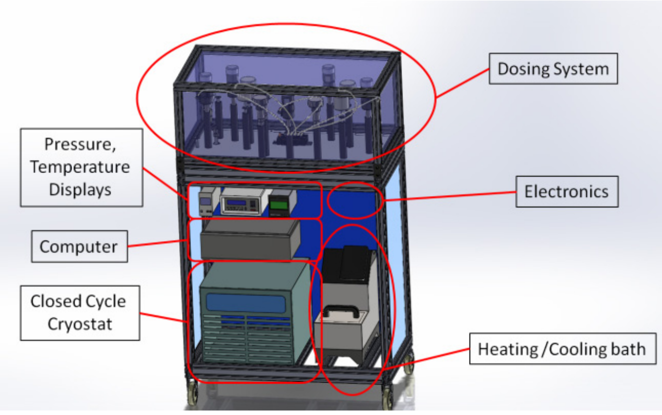

***Figure 3** Dosing system with controlling electronics, pressure gauges and temperature controls*

Fig. 1 shows the control unit with the gas dosing system (manyfold), cooling units and electronics. The dosing system consists of a special arranged pneumatic valve combination that allows to control the gas supply into the sample in two different ways. On the one hand, the sorbent can be dosed stepwise into the sample chamber to reach equilibrium states at a certain gas pressure, allowing to quantitatively calculate the adsorbed amound for quantitative sorption isotherms. On the other hand, continious dosing is also possible via a proportionality valve.

One of the most important sorbents for physisorption experiments is nitrogen due to its small molecule size and weak interaction with most materials. This allows to use the BET method to determine the total surface area and the porosity of the material investigated. The use of Nitrogen requires temperatures of 77K and the sample holder needs to be cooled down to this temperature which is achieved with a He closed cycle cryostate. As in the SAXS setup space is quite limited, the size of the sample holder has to be as small as possible but still has to contain a sample of several millimeters diameter.
Fig. 2 shows the design of the sample holder, which consist of two cylinders covering the sample. The outer cylinder (Fig. 2a) is responsible to provide a evacuated shielding to avoid vapor condensation on the elongation of the coldfinger and to reach temperatures beneath 77K. The inner cylinder coontains the sample and keeps the space filled with the sorbent as small as possible, so that background from the scattered X-rays by the sorbent gas is minimized.

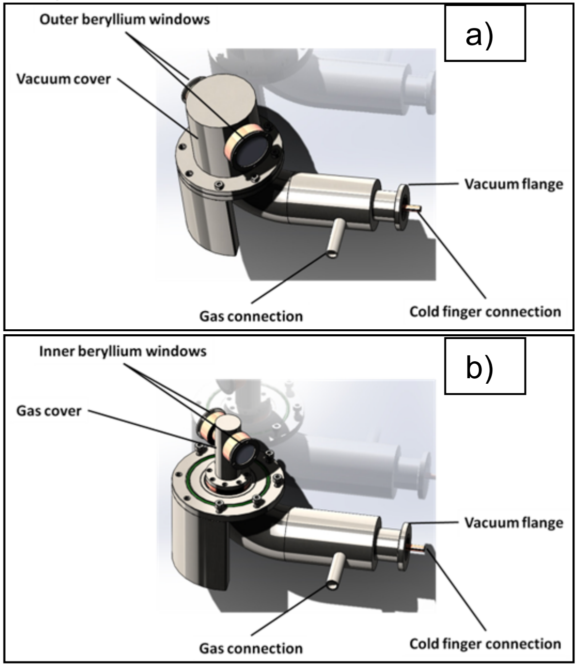

***Figure 4** Sample holder with cold-finger connection and gas inlet*

The whole system is designed to be implemented into the N8 Horizon SAXS instrument. However, the modular construction will make it eligible also for other SAXS systems like the NanoStar or for use at synchrotron radiation beamlines with only slight adaptations.
The system is currently under development and will be fully operational by end 2016. Applications as described in the above reports (e.g. sorption induced deformation) will thus also be feasible with laboratory SAXS systems.

2) In-situ SAXS during charging/discharging energy storage devices

If electromagnetic radiation like X-rays hits a material part of the intensity is absorbed by the material. The amount absorbed depends on the concentration and type of elements within the material. We have used this principle for the first time to study concentration changes of cations and anions in electrical energy storage devices (supercapacitors, see previous report) quantitatively.

To achieve this, we have developed a special in-operando supercapacitor cell, where only one electrode at a time is hit by the x-ray beam. This cell allows the independent measurement of cation and anion fluxes during charging and discharging on every conventional X-ray scattering system with an attached Potentiostat. As indicated in Fig. 3 (top) a hole in all cell components, except of the working electrode ensures the study of ion electrosorption within this electrode only. While applying various voltage signals to the electrode via the Potentiostat, the change in the transmitted beam intensity is recorded via the “Glassy Carbon” method. For this a strongly scattering glassy carbon sample right after the in-situ cell produces a homogenous scattering pattern on the 2D SAXS detector, its total intensity being proportional to the beam transmitted through the working electrode. Simultaneously the current is tracked by the Potentiostat (see Fig. 3), which is needed as additional input for the calculation of both cation and anion concentration changes [1].

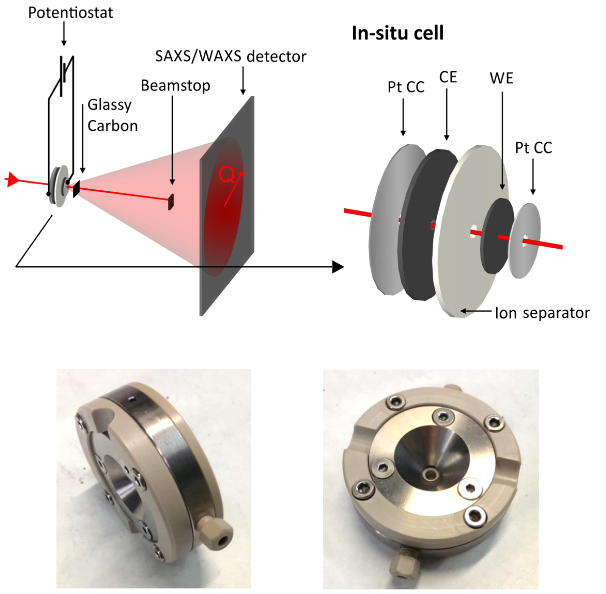

Figure 3: *Top: Sketch of the experimental set-up and the multi-layered assembly of the in-situ supercapacitor cell. Bottom: photo of the in-situ cell.*

Our results indicate that the way how electrical energy is stored within nanoporous carbons is different from traditional views. In Fig. 4a possible mechanisms how ions could contribute to charge storage are indicated. From X-ray transmission we found, that beside counter-ion adsorption also co-ion expulsion contributes significantly to ion electrosorption leading to so-called ion swapping (Fig. 4a (iii) and b). This was shown for the first time using aqueous electrolytes with high ionic strength. In combination with in-situ small-angle x-ray scattering (SAXS) measurements at large scale research facilities (synchrotron radiation sources) an in-depth picture of the ion structure could be derived [1].

Understanding how many and which ions are going where as a response to an applied voltage allows the direct prediction of an optimized porous electrode material.

Conventional electrochemical techniques usually track the current-voltage characteristics of such devices. Since the measured current is accommodated by electrons or holes within the electrode all information about positive and negatively charged ions within the electrode pores is indirect. In-situ x-ray transmission is a simple way to directly probe cation and anion concentration changes within an in-situ supercapacitor during electrochemical cycling. These measurements can be set-up in virtually any commercial x-ray diffraction and scattering system, and are therefore believed to find widespread applications for in-situ electrochemical measurements.

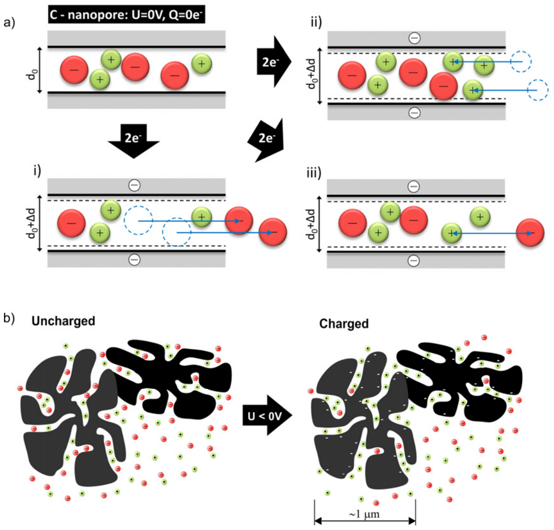

Figure 4: *a) The sketch visualizes the different possibilities how ions can counterbalance the electrode charges in a slit-like pore. Our experiments have shown that ion swapping is the main mechanism of charge storage.*

3) 2D-Indirect Fourier-Transformation

Scattering experiments require some kind of model for data interpretation. The selection of the correct model can be difficult, since the measured scattering pattern is in reciprocal space and typically it is easier to think in terms of real space.

The indirect Fourier transformation can be used to transform the scattering data from reciprocal into real space. The resulting pair distance distribution function (PDDF) contains the same information as the original scattering dataset, but its information can be interpreted more directly due to its real space representation. The technique has been established in the late 1970s for one dimensional scattering curves. It has been extended to 2D scattering patterns a couple of years ago [2].

In order to use the two dimensional Fourier transformation efficiently, it is helpful to deduce some simple rules to relate its properties to parameters describing the structure. This pertains to size, shape and internal architecture of the structures.

One simple rule of the one dimensional case is for example that the point, where the PDDF reaches zero corresponds to the maximum dimension, found in the structure. Similarly, in the two dimensional case, the contour line, where the PDDF reaches zero corresponds to the maximum distance found within this structure in this direction. If the projection of the structure onto the detector plane is a convex set with two fold symmetry, the shape of this contour line directly represents the shape of the structure, and the size is just increased by a factor of two. This holds for many common structures, like cylinders, ellipsoids, and cuboids. Therefore, the length and the diameter of a cylinder can be determined directly as well as the half axes of an ellipsoid.

Additional rules can be deduced, for cuts through the PDDF. They allow e.g. for determination of core size and shape of a core-shell structure.

Fig. 5 gives an example for the interpretation of the two dimensional PDDF [3]. The sample is porous silica templated by normal wood. The indirect Fourier transformation results in a function that shows two bars. The two bars correspond to two layers within the cell wall, where the pores are oriented in different directions. These differently oriented pores cannot be intermingled in one layer, since the PDDF is just the sum of two convex sets without cross terms. The vertical bar is dominant since it originates from the thickest layer within the cell wall. Relating the height of the two bars, one can therefore estimate the thickness of the cell wall layers. The width of the vertical bar is about 16 nm, and a length of about 80 nm. Half of the length is 40 nm, which corresponds to about the resolution of the instrument and is therefore the minimum length of the structures.

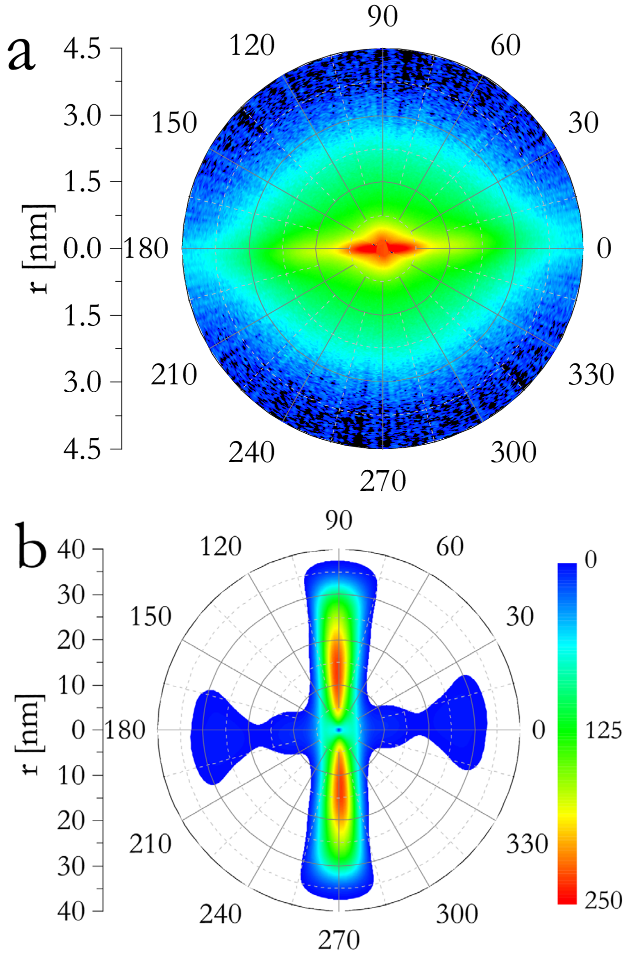

***Figure 5**: (a) Scattering pattern of porous silica templated by wood, and (b) the corresponding two dimensional PDDF.*

Half of the width is 8 nm, which is the diameter of a microfibril replicated in silica. Its shape is slightly bent outwards, which one can use to measure the microfibril angle directly.

All these and some additional parameters obtained from cuts through the function can be used to develop a rather detailed model of the structure.

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Cooperation

- Lutz Brügemann, (Bruker AXS Karlruhe)
- Günther Maier (Materials Center Leoben)

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Nanomaterials & Scattering

Computational Materials Physics

Markus A. Hartmann, Soran Nabavi, Oskar Paris
markus.hartmann@univie.ac.at

The microscopic mechanisms during the deformation of nanomaterials are hard to grasp experimentally. This is especially true in highly complex biological materials as well as in carbon nanostructures. Both material classes promise to help in developing new high performance materials. In our group we use the numerical power that modern computers provide to perform computational mechanical tests on such complex materials using simplified atomistic model systems. We use Monte Carlo methods to gain fundamental understanding of the complex microscopic deformation behavior of modern materials. The investigated systems are motivated by reversibly cross-linked polymeric materials as well as by carbon nanostructures like graphene, carbon nanotubes, and fullerenes.

1) Reversibly cross-linked polymers

In the framework of the FWF funded project P-22983-N20 the influence of reversible cross-links on the mechanical behavior of polymeric structures was investigated. This work is motivated by the concept of sacrificial bonds that can be found in a large variety of biological materials, like bone, wood, silk or the mussel byssus. Upon loading it is first the weak cross-links that fail, before the covalent backbone of the structure ruptures. Consequently, the previously shielded parts of the polymer may extend revealing the so called *hidden length*. This mechanism is highly effective in dissipating energy. Because the cross-links are reversible they re-form after the load was released giving the system self healing capabilities.

A simple model containing reversible cross-links was investigated (see Figure 1). In [1] the influence of the type of topology on load-displacement curves for single chains was studied. Figure 2 shows some of the obtained results. Although the number of cross-links is the same in all three investigated structures the load-displacement curves show remarkable differences that can be attributed to the different topologies investigated. The work to fracture increases by a factor more than two for the nested and pseudo-knotted structure compared to the independent topology. Also the amount of dissipated energy is smaller for the independent topology as compared to the other two topologies. A very interesting feature of the load-displacement curves is that the sacrificial force peaks show different heights (corresponding to different strengths) although the cross-links are energetically equivalent. This is due to entropic effects stemming from backbone fluctuations that depend on the end-to-end distance of the chain.

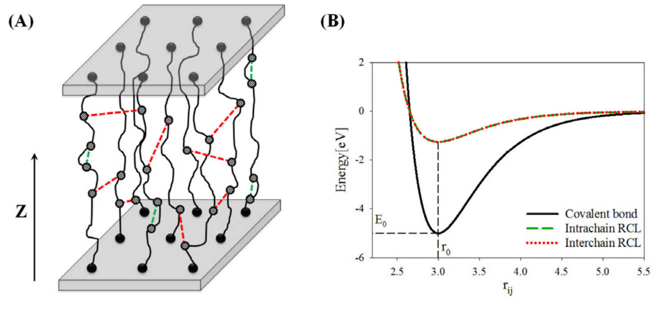

Figure 1: *The model used to investigate the effect of reversible cross-links on aligned fiber bundles. The chains were permanently grafted on two impenetrable plates. Cross-links were allowed to form connecting beads of the same and of different chains, respectively.*

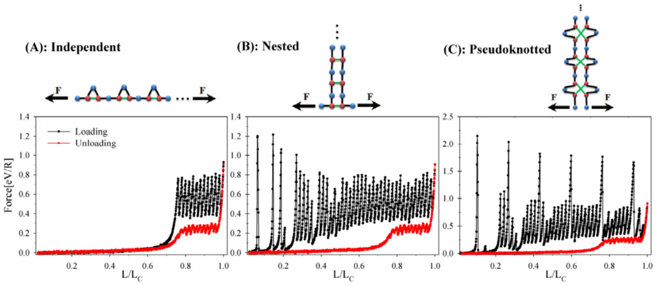

Figure 2: *The influence of cross-link topology on the resulting load-displacement curves. The three investigated topologies (top row) show remarkable differences in the load-displacement curves (bottom row). One key parameter is the dissipated energy given by the hysteresis area between the loading- and unloading curve [1].*

In [2] the model was extended to investigate not only single chains but also cross-linked chain bundles (see Figure 1). The main difference is that cross-links may now also form between different chains altering dramatically the mechanical behavior. One prominent effect is that inter-chain cross-links may decrease the effective strength of an aligned fiber bundle due to a premature rupture of the polymer backbone. Figure 3 explains this effect. In the case of a single chain the strength of the backbone can only be exceeded by the cooperative, parallel loading of 5 or more cross-links (A). In the case of two or more chains only two cross-links are sufficient to rupture the backbone of the polymer (B). It could be shown that this effect is strongly dependent on the grafting density.

In November 2014 S. Soran Nabavi successfully defended his PhD thesis *Reversible cross-links in polymer chains*.

2) Mechanical properties of carbon nanostructures

Unique electronic and mechanical properties make carbon a possible candidate to revolutionize electronics as well as structural mechanics. To fully exploit the potential of carbon nanostructures it is necessary to understand their deformation behavior from a fundamental point of view. Together with colleagues from Montanuniversität Leoben and the Vienna

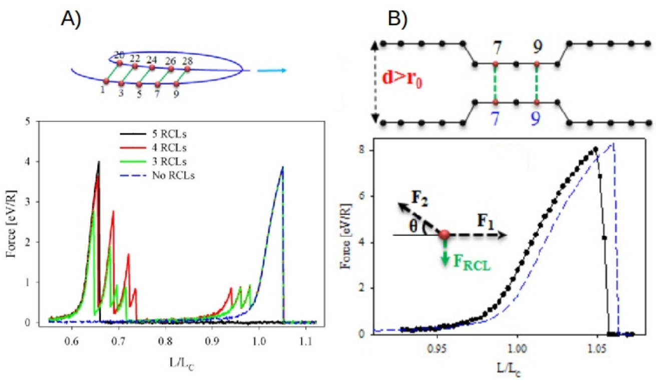

Figure 3: *(A) shows for a single chain a topology of cross-links that exceeds the strength of the backbone. Here 5 cross-links are loaded in parallel. (B) In the case of two or more chains only two inter-chain cross-links are sufficient to rupture the backbone of the structure. This effect is strongly dependent on the grafting density of the structure [2].*

University of Technology we studied the mechanical behavior of different carbon nanostructures over many different length scales employing a variety of different methods ranging from atomistic *ab initio* and Monte Carlo methods to continuum mechanical Finite Element calculations. The strategy is to use *ab initio* calculations to determine classical potentials that can be used in Monte Carlo simulations. In the Monte Carlo simulations computational mechanical tests are performed to obtain effective mechanical parameters of the material that can be used in continuum mechanical calculations of larger structures. Special emphasis is put on the mechanical stability of these structures. Figure 4 shows the obtained results for carbon nanotubes of different radii and chirality that were loaded hydrostatically. The figure shows the critical pressure (i.e. the onset of ovalization of the cross-section) (top) and the bulk modulus (bottom). The bulk modulus is defined as the pressure per volume change $p=-K(\Delta V/V_0)$. The solid lines are predictions from shell theory for loading of thin cylinders. The lines are not fits to the data, but obtained from the elastic modulus $Y=313$ N/m, the Poisson ratio $n=0.18$ and the thickness $h=1.32$ Å of monolayer graphene that was obtained independently [5]. The figure shows that the bulk modulus is accurately described by the continuum mechanical model for nanotubes of armchair as well as zigzag type for all sizes investigated. The critical pressure is less well predicted. For small sizes of the armchair type the critical pressure may even be overestimated several orders of magnitude.

A treatise covering some of the aspects on atomistic and continuum mechanical modeling of carbon nanostructures that evolved from a series of lectures given by M. A. Hartmann in the framework of a CISM lecture in Udine, Italy, in July 2014 is given in [4].

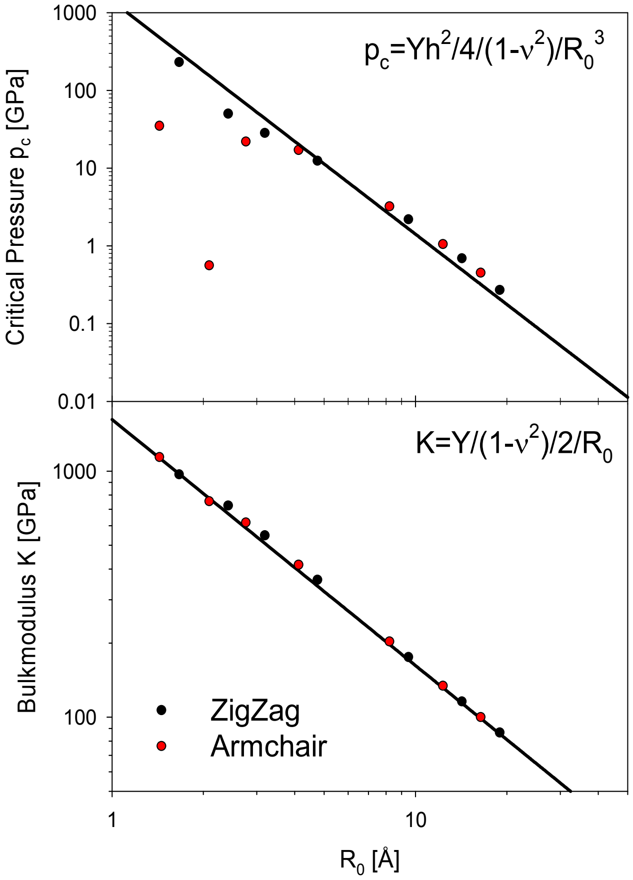

Figure 4: *Critical pressure and bulk modulus for nanotubes of different sizes and chiralities. Solid lines indicate continuum mechanical predictions for thin walled cylinders. These are are obtained by using the elastic constants of monolayer graphene that were obtained independently.*

Funding

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Cooperation

- M. J. Harrington, P. Fratzl (Max-Planck-Institute of Colloids and Interfaces, Potsdam)
- M. Todt, F. G. Rammerstorfer (ILSB, Vienna University of Technology)
- Y. Sun, D. J. Dunstan (Queen Mary University, London)
- D. Holec, F. D. Fischer (Montanuniversitaet Leoben)

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Nanomaterials & Scattering / Surface Physics & Scanning Probe Microscopy

Bioinspired Actuators

Gerhard Fritz-Popovski, Christian Ganser, Roland Morak, Christian Teichert, Oskar Paris
gerhard.popovski@unileoben.ac.at
oskar.paris@unileoben.ac.at

1) Moisture driven ceramic bilayers from biotemplating of pine cones

Pine cones open and close depending on humidity. Since there is no active metabolism in the scales, the movement depends on the material properties. This material consists like wood of cellulose elementary fibrils that are aligned in parallel. Several of these elementary fibrils form together with hemicelluloses as matrix a bundle called microfibrils. Between the microfibrils there is lignin. Native cone scales consist of two layers in the region that causes the movement, namely the so-called “fibre layer” close to the axis of the cone and a “sclerid layer” at the outer side. The two layers differ in their microfibril angle, *i.e.* the angle of the microfibrils relative to the central axis of the elongated cells. Since the cells are oriented roughly in parallel to the centre axis of the scale, the microfibrils of the fibre layer are also oriented parallel to the scale axis, while those in the sclerid layer are normal to the scale axis. Water is adsorbed preferentially in the matrix between the elementary microfibrils leading to matrix swelling, while the embedded microfibrils represent a stiff, non-swellable backbone (Fig. 1a). The direction of swelling is therefore different for the two layers, which leads to a deformation of the scale similar to a bimetallic strip.

Such cones can be replicated in silica using an approach similar to the replication of wood [1]. The inorganic precursors penetrate preferentially the matrix, but hardly the cellulose elementary fibrils. Calcination leads therefore to a templated material that consists of silica, where the swellable hemicelluloses used to be in the scales, and pores, where the elementary fibrils used to be. The layered architecture of the scales could be replicated as seen in the position resolves small angle scattering experiment (Fig. 2), which was performed at the synchrotron radiation source BESSY II in Berlin. The former fibril and sclerid layers can clearly be distinguished in the silica material by the different orientation of the nanostructures found. The replicated structures show typical sizes on the order of a few nanometres. The replicated cone scales were found to show humidity dependent movements. Changing from dry to humid conditions leads to a “closing” of the replicated cone and subsequent drying is followed by an “opening”. Although the measured angular movement is only a few degrees of arc, the replicated materials clearly shows humidity induced actuation into the very same direction as the original biological template. The actuation *mechanism* must however be different from the native structure, since the nanoporous silica-cone has no more swellable matrix and no stiff elementary fibrils.

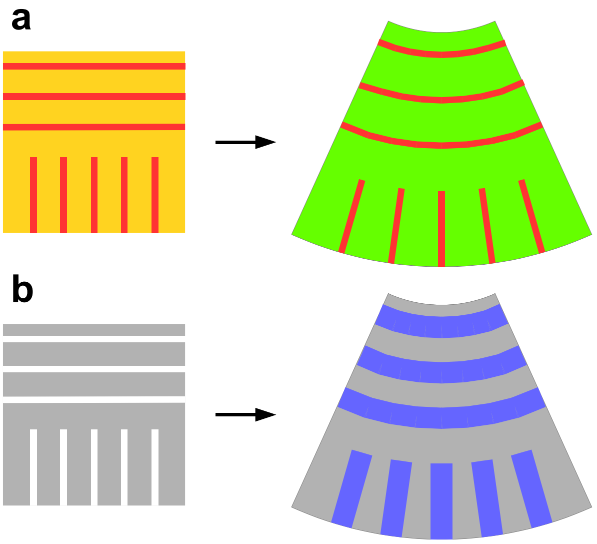

***Figure 1**: (a) Opening mechanism of native pine cone. Microfibrils (red) embedded in a dry matrix (yellow) and in a wet matrix (green). (b) Empty pores (white) within a silica matrix (grey) and water filled pores (blue)*

It is well known that liquid uptake alters the surface energy of the pore walls (see the following report on fluid sorption in nanoporous materials). This energy change, as well as the curvature of the liquid film and capillary pressure of the hemispherical menisci at the pore ends at capillary condensation lead to stresses and related strains in the pore walls, and thus, to deformation of the porous material. For long cylindrical pores, this deformation can be expected to be anisotropic, having different effects for the two layers of the scale. Assuming that only the pore diameter changes upon water uptake, such a mechanism will also lead to a movement of the whole scale as sketched in Fig. 1b. An idealised model for such a type of bilayer bending due to pore swelling (see below) for the given materials and pore sizes can be used to theoretically estimate a bending by 1.3°±0.6°. Given all uncertainties, this agrees reasonably with experiment where we observed 2.8°±0.6° [2].

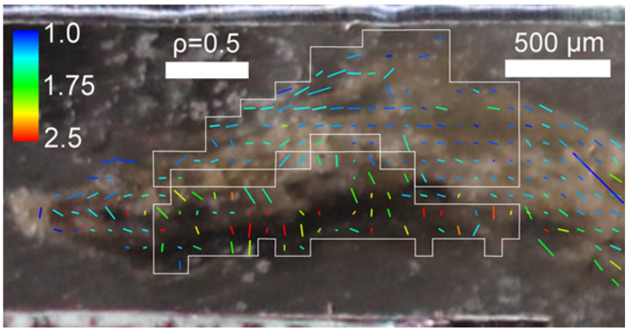

***Figure 2**: Position resolves small angle X-ray scattering results. The direction of the lines gives the orientation of the nanostructures (i.e., the pores), and the length is a measure for the amount of oriented nanostructures. Colours give their mean cord length. The white lines indicate the fibre layer (top) and the sclerid layer (bottom) of the active region.*

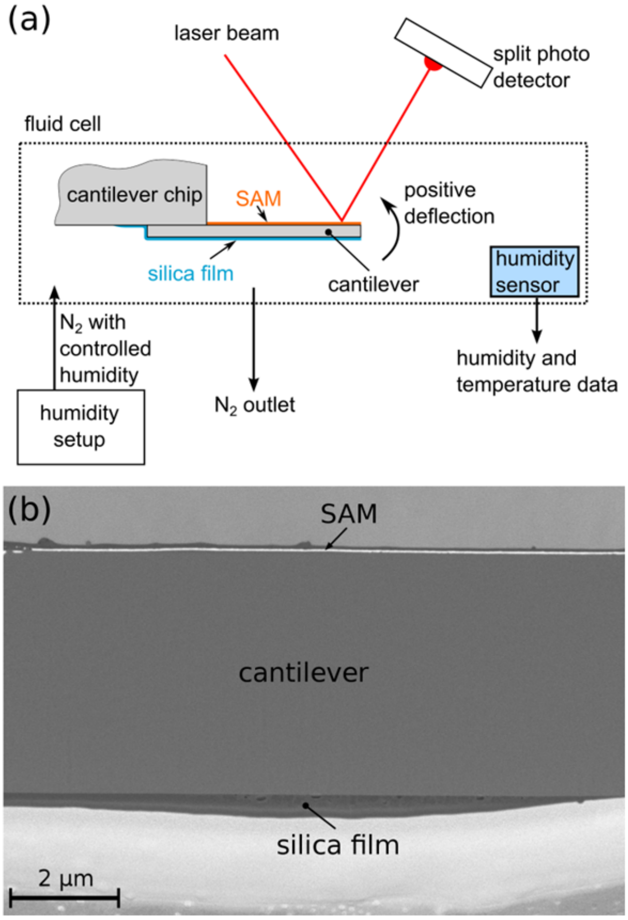

Figure 3: *(a) Schematic representation of the experimental setup. (b) SEM image of cantilever cross section with Au-coating and a hydrophobic SAM layer on top and the mesoporous silica layer at the bottom.*

2) Microcantilever actuators based on nanoporous silica / silicon bilayers

The actuation principle of the replicated pine cone can be transferred to biologically inspired actuators. The basic idea consists in a layered structure, where the liquid sorption in pores leads to different deformation of the two layers. Since it is not necessary to have two porous layers, the simplest realization of such a system is to combine a solid (non-porous) layer with a nanoporous one. This was achieved by using a commercially available cantilever for atomic force microscopy (AFM), whose deflection can be monitored with high accuracy using the AFM read-out system. The cantilever was coated with a layer of ordered mesoporous silica, synthesized via a soft templating approach by evaporation induced self-assembly after dip coating. Since a bending movement is only possible if the porous layer is just on one side of the cantilever, the Au-coated side of the cantilever was modified by a hydrophobic self-assembled monolayer (SAM). This prevents the formation of a silica film on this side of the cantilever on the one hand, and the reflective Au-coating can still be used for read-out on the other hand (Fig. 3).

A cantilever prepared in this way shows a positive deflection upon humidity increase (Fig. 4, left). Reducing the humidity again leads to desorption of the water and the cantilever returns back to its original state. The observation of the macroscopic movement can be compared with the microscopic humidity induced strain. The pores within the silica film are cylindrical and ordered on a rectangular lattice with the cylinder axis parallel to the surface (for details, see the following report “fluid sorption in nanoporous materials”). Therefore, the microscopic strain can be obtained from the shift of the Bragg reflections from the ordered mesopores by employing in-situ grazing-incidence small-angle X-ray scattering (GISAXS), which were performed at the Austrian SAXS beamline at the synchrotron radiation source ELETTRA in Trieste. The pore lattice strain (Fig. 4, right) shows a similar humidity dependence as the cantilever deflection. Indeed, bilayer bending theory predicts for the given system (given geometry and layer materials) a linear relationship between the cantilever deflection and the strain difference between the two layers.

A more fundamental understanding of the sorption induced deformation leading to active movement of the devices reported here will be discussed in more detail in the following report. The combination of a rigorous thermodynamic model for the pressure in the pores from literature combined with elasticity considerations for simple pore geometry yield a quantitative model predicting the cantilever bending. Interestingly, within some limits this model depends only on the geometry of the cantilever, the pore surface to volume ratio, and the Youngs modulus of the substrate, but not on the

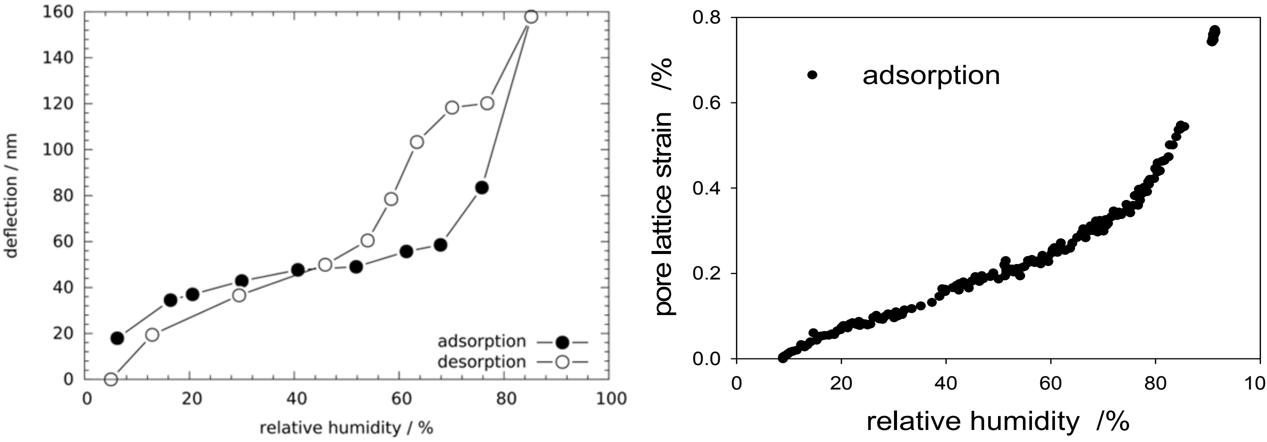

Figure 4*: Deflection of the cantilever during a sorption cycle (left) and deformation of the pore lattice determined from the out-of-plane 02 reflection (right)*

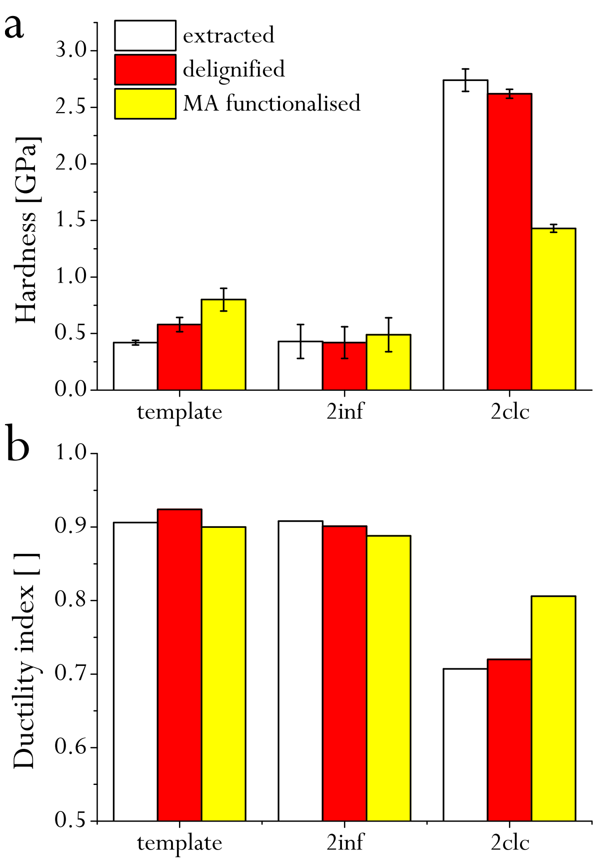

***Figure 5**: (a) Hardness and (b) ductility index of wood, delignified wood and woof treated with MA. The samples were taken as such (template), twice infiltrated with TEOS (2inf) and calcinated (2clc)*

mechanical properties of the porous film. The calculation yields a deflection of 86 nm, which is in good agreement with the observed value of 140 nm, taking all simplifications into account [3]

3) Passive mechanical properties of silica templated by wood

Besides the active mechanical properties reported above, biotemplated materials can exhibit also interesting passive mechanical properties, such as a quite high ductility despite of being ceramics. As already reported earlier [1], wood can be used as a template for its replication into silica on length scales from macroscopic dimensions down to a few nanometres. A detailed replication is, however, only possible if the inorganic precursor molecules can penetrate well into at least some of the biopolymers forming the cell walls. This can be achieved by delignification followed by a treatment with maleic acid anhydride before impregnating the silica precursor. Subsequent drying and calcination results in a highly porous material that retains the entire nanostructure of native wood. Here, the mechanical properties of the cell walls determined by nanoindentation are reported [4].

The hardness (Fig. 5a) of wood is not changed much by the deliginification step or by the treatment with maleic acid anhydride (MA). Infiltration with the precursor molecules also leaves the properties basically unaltered. As expected, calcination leads to a strong increase in hardness (and similar in Youngs modulus, not shown). The hardness is, however, still much lower than the value of 6.3 GPa reported for fused silica. If one compares the values found for replicas prepared from essentially untreated wood (termed “extracted”), from delignified wood and from wood after delignification and MA treatment, the hardness of the sample templated by the MA treated wood is significantly lower. One might suppose that the lower hardness found for this sample might be just due to a higher porosity. The porosity of the cell walls can be estimated from N_2 sorption experiments. If one rescales the hardness simply linearly by the amount of empty space, one obtains higher values than the ones in Fig. 5a, but still much lower than for fused silica. In addition, the rescaled hardness of the MA modified templated sample is still only 2/3 of the hardness of the other silica replicates of wood.

Very interestingly, the ductility index (Fig. 5b), which is a measure for the energy stored in the system due to irreversible deformation, only decreases gently after calcination. Here, the MA functionalized material clearly outperforms the two other samples. The low hardness and the high ductility index suggest that in particular the material templated by the MA modified wood can take up a considerable amount of energy by an irreversible deformation mechanism. This mechanism is presumably based on the collapse of small pores, which hinders crack propagation and leads to a high fracture toughness of the material.

Funding

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Cooperation

- 1) & 3) C. Zollfrank, D. Van Opdenbosch (TU München), W. Wagermaier, (MPI Golm),
- 2) Heinz Amenitsch, Benedetta Marmiroli, Barbara Sartori, (TU Graz and SAXS beamline, ELETTRA Trieste); Annelie Weinberg, Lisa Martinelli (Med. Univ. Graz), Thomas Griesser (MU Leoben)
- 3) Thomas Schöberl (ESI Leoben).

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Surface Physics & Scanning Probe Microscopy

Cellulose based materials

Christian Ganser, Patrice Kreiml, Caterina Czibula, Christian Teichert
teichert@unileoben.ac.at

Cellulose based materials are present in a variety of forms in modern society. Starting with wood as a construction material, via paper as an information carrier, to textiles and hygiene products, a broad range of applications is covered by this class of materials.
The work presented in the following was conducted within the Christian Doppler Laboratory for “Surface Chemical and Physical Fundamentals of Paper Strength”, coordinated by Prof. Robert Schennach (Graz University of Technology).

1) Humidity influence on mechanical properties of cellulose materials

Cellulose materials are, in contrast to most engineering materials, hydrogen bonded and thus subject to significant change of mechanical properties upon water uptake. Using atomic force microscopy based nanoindentation (AFM-NI) [1,2], the decrease of viscose fibers’ mechanical properties – hardness H and reduced Modulus E_r – was monitored as a function of relative humidity φ_r [3,4]. As is visible from Fig. 1, the depth and lateral size of the residual indents increased with increasing humidity, already indicating a decrease of hardness.

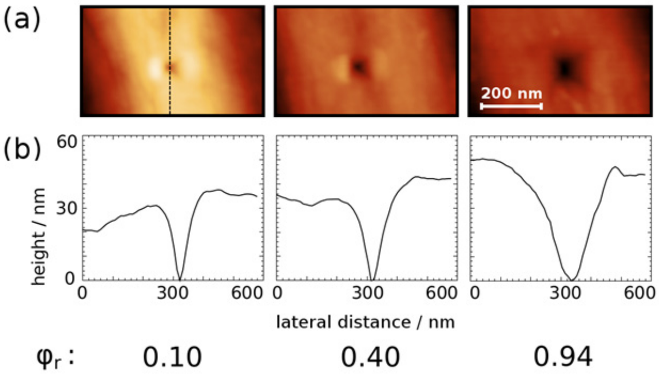

Figure 1 *AFM images of indents on a viscose fiber at different relative humidities φ_r (a) and height profiles across the indents (b). (From [3].)*

Using the adsorption measurement from Fig. 2, the viscose fibers’ water uptake could be related to the relative humidity of their environment.

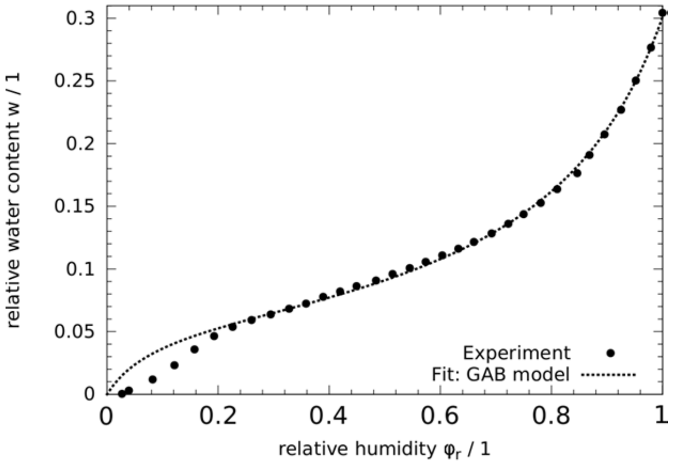

Figure 2 *A viscose fiber’s water uptake as a function of relative humidity. (From [3].)*

In Fig. 3 the mechanical properties H and E_r are both plotted against the fibers’ relative water uptake. Note that even at $\varphi_r = 1$ (relative water content ≈ 0.3), fairly high values of H and E_r are expected.

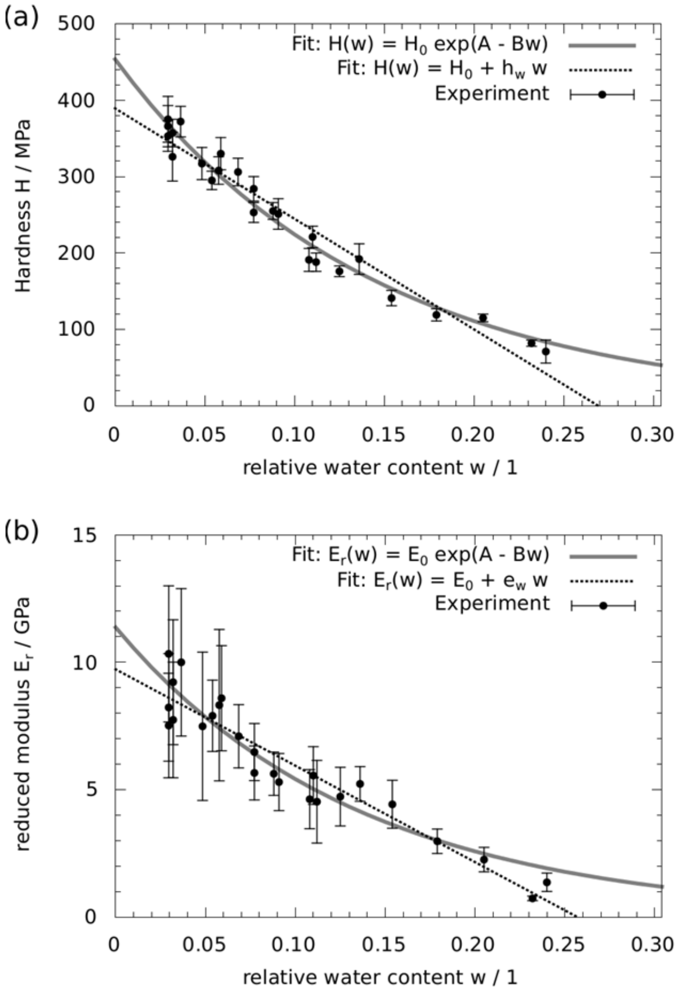

Figure 3 *Hardness (a) and reduced modulus (b) of a viscose fiber as a function of water uptake. (From [3].)*

When a viscose fiber is swollen in water for several hours, its hardness and reduced modulus values are decreased further by factors of about 4 and 20, respectively. [3,4]

2) Water uptake behavior of cellulosic fibers

Cellulose fibers for textile or hygiene applications are often required to excel in water uptake capacity. However, small variations during the production process can change the water uptake of these fibers significantly. In order to find the reason of such variations AFM topography measurements of fibers with different water uptake behavior were performed. Two sets of fibers with “good” and “bad” water uptake capacities were analyzed. Surface roughness did not indicate any differences between the fibers. Interestingly, trenches on the fiber surfaces were found (see Fig. 4), which appeared to be linked to the water uptake capacity of the fibers. To analyze the trench density, a MATLAB program was devised which allowed a fast and precise processing of the AFM topography images. In the first set of samples, a significant difference in trench density was found between “good” and “bad” water uptake. In the second set, the difference was less significant. If a link between surface features and water uptake behavior is present, the trenches are the most likely indicator. [5]

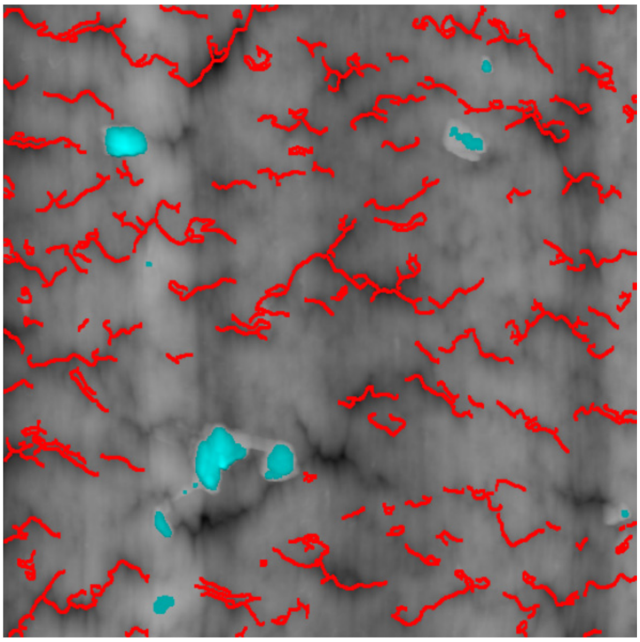

Figure 4 *Surface trenches on a viscose fiber (marked in red). (From [5].)*

3) Evaluation of AFM force mapping to study rough xylan-cellulose films

Wood is a composite of cellulose, hemicellulose, and lignin. In order to understand all processes in papermaking, it is of interest to localize all three components on a pulp fiber surface. One idea to achieve this, are AFM force maps, where the adhesion force between tip and surface is recorded at each point of the map. For this purpose, a model system was devised: xylan precipitates on a cellulose substrate. This system exhibits a rough surface, which is also the case for pulp fibers. First trials looked promising [6]. However, the results of force mapping showed that it was not possible to measure the adhesion force properly. The reason is that the surface morphology is influencing the contact area between tip and sample, which in turn influences the measured adhesion forces. By comparing Fig. 5a with 5b, it is evident that a low adhesion force is measured on elevated areas and a high adhesion force at surface depressions.

This study leads to the conclusion that in order to make significant assertions of adhesion forces from AFM force mapping, it is most important to correct for the topography induced contact area.

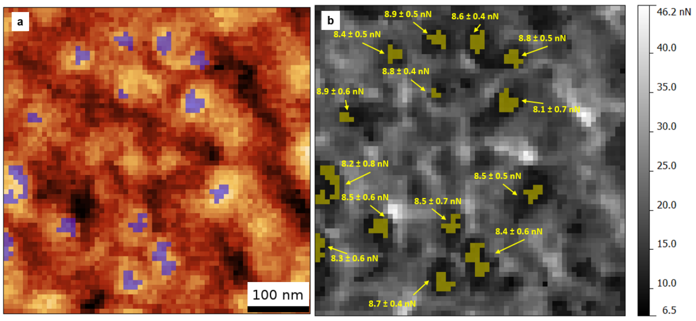

Figure 5 *Maps of (a) topography (z-scale:15 nm) and (b) adhesion force for a cellulose film with adsorbed xylan.*

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Christian Doppler Laboratory for “Surface Chemical and Physical Fundamentals of Paper Strength”

Cooperation

- Robert Schennach, Frederik Weber, Sebastian Rohm (Institute of Solid State Physics, Graz University of Technology);
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- Stefan Spirk (Institute for Chemistry and Technology of Materials, Graz University of Technology and Institute for the Engineering and Design of Materials, University of Maribor);
- Walter Roggenstein, Ingo Bernt (Kelheim Fibres GmbH);
- Leo Arpa, Franz J. Schmied (Mondi Frantschach).

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Surface Physics & Scanning Probe Microscopy

Investigating electronic/ electrochemical properties using advanced atomic force microscopy

M. Kratzer, M. Huszar, C. Teichert
Markus.Kratzer@unileoben.ac.at

Photoconductive AFM and Photo-assisted Kelvin Probe Force Microscopy on radial junction solar cells

A novel type of solar cells can be realized by using so called radial junctions. Here such radial junctions are realized by using p-doped silicon nanowires (NW) which are coated by undoped amorphous silicon and then covered by a thin layer of n-type amorphous silicon. The NWs are grown on a transparent conductive metal oxide electrode to enable illumination. It has been shown that the RJs exhibit an inhomogeneous distribution of the local conductivities. The effect of these inhomogeneities on the integral solar cell performance is vastly unknown.

In order to gain deeper insight a comprehensive atomic force microscopy based study on the electrical and morphological properties of RJ solar cells has been performed. Especially photo-conductive atomic force microscopy (PC-AFM) and photo-assisted Kelvin probe force microscopy (PA-KPFM) measurements are perfectly suited for the nanoscale electrical characterization. PC-AFM provides information of the local photo-current and PA-KPFM gives insight in the local surface photo-voltage generation. It is important to get the corresponding information from the same areas in order to draw meaningful conclusions. Therefore, a procedure has been developed to relocate certain areas and perform the complementary measurements at the exactly same positions.[1]

The areas are marked by a nanoindentation imprint. This way the marks can be used for repositioning of the AFM scanner. In Fig 1 a current map (C-AFM) and the corresponding contact potential difference map (KPFM) from the same position are shown. Inhomogeneities in the electrical behavior are visible for both, current and KPFM signal. Interestingly the inhomogeneities do not necessarily coincide suggesting that there exist different meachnisms that cause the inhomogeneities.

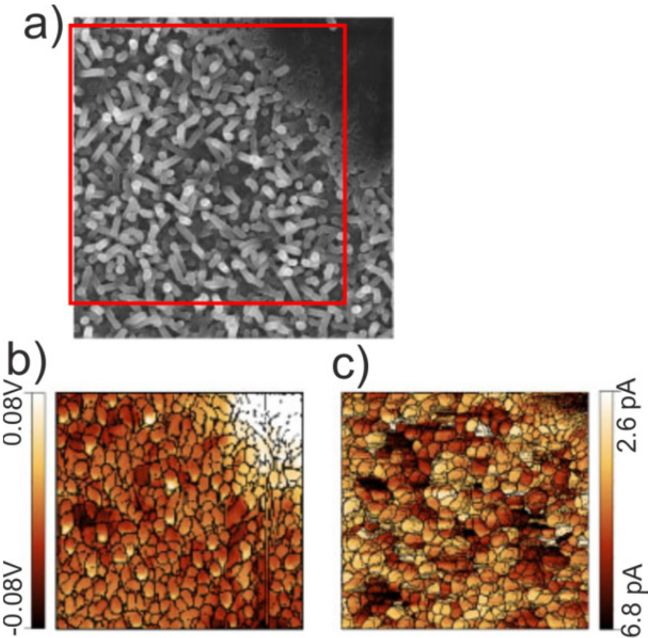

Figure 1: *a) SEM image of the NW covered surface. On the top right the nano-indent is visible. in b) and c) the corresponding KPFM signal and (photo) current maps are shown. The area of measurement is indicated by the red square in a) (From [2]).*

Investigating corrosion processes on Al-alloys using KPFM

The ability to map variations in the local surface potential makes KPFM also suitable for the investigation of corrosion processes. High strength aluminum brazing compounds as used in car-cooler systems tend to corrode after brazing. Therefore, an intermediate layer is inserted to separate the 4xxx filler-material from the 7xxx base-material. The effectivity of this inter-layer in preventing corrosion was investigated using KPFM. The samples were subjected to a simulated brazing cycle and exposed to a corrosive medium. The measurements indicate the presence of cathodic inclusions in the Al-matrix. Further, a line of up to 3 µm wide holes is formed at the transition between intermediate layer and base material. In Fig 2, a KPFM map of the transition area between an AlMn (left part of the image) layer and the $AlZn_{4.5}$ Mg base material (right part of the image) after being subjected to a 42 g/l NaCl solution at pH 3 for 1 hour is shown.

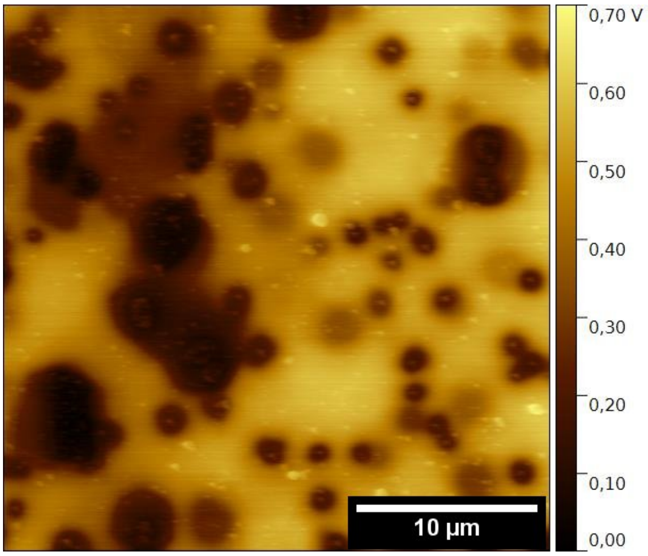

Figure 2: *KPFM map of the transition region between the base material (AlZn4.5Mg) and AlMn interlayer after 1 hour exposure to NaCl solution.*

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Cooperation

- Fejfar, M. Hyvl, A. Vetishka Institute of Physics, Academy of Sciences of the Czech Republic, Praha, Czech Republic.
- T. Kremmer, M. Huszar, H. Antrekowitsch: Chair of Nonferrous Metallurgy, MU Leoben, Leoben, Austria

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Surface Physics & Scanning Probe Microscopy

Organic thin film growth on atomically flat and rippled TiO_2(110) substrates.

M. Kratzer, J. Genser, C. Teichert
Markus.Kratzer@unileoben.ac.at

Controlling the growth of thin films of conjugated organic molecules is a key issue in organic electronics. Here, we report on the growth of the organic semiconductor para-hexaphenyl (6P) on flat and ion-bombarded rippled TiO_2(110) surfaces.

Flat, atomically clean TiO_2(110) [1]

Smooth, rutile TiO_2(110) surfaces have been prepared by annealing and ion bombardment cycles under ultra-high vacuum conditions. Deposition of 6P using organic molecular beam epitaxy (OMBE) on freshly prepared flat TiO_2 resulted in the formation of elongated bunches of needles consisting of flat lying molecules. The needles' long axes point towards the [1-10] direction.(Fig 1) This means that the molecular long axes are aligned with the [001] direction parallel to the oxygen rows of the TiO_2(110) surface. The formation of needle bunches can be explained by an enhanced nucleation probability in the vicinity of already existing nano-needles due to an locally increased molecular density arising from the tailback of molecules that could not be incorporated into the needle. Exposing the thin films to ambient air induces the formation of small entities which are most likely formed at the cost of a compact 6P wetting layer remaining in the needle free areas. Air exposure or roughening of the surface by ion beam bombardment prior to deposition leads to the formation of dendritic islands composed of upright standing molecules. In this case no evidence of a wetting layer can be found.

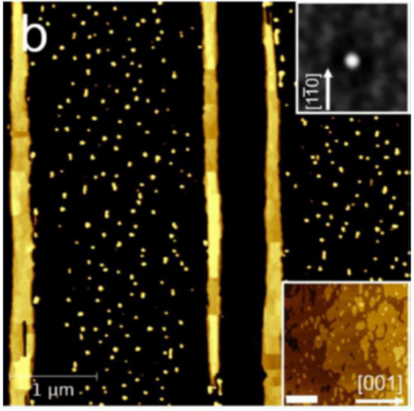

Figure 1: *AFM topography image of nanoneedles pointing in the [1-10] direction and small 6P entities formed by the air induced decomposition of a 6P wetting layer. Right top corner: 2D autocorrelation function of an area without needles. Right bottom corner: STM image of the pristine surface prior to deposition (From [1]).*

Rippled TiO_2(110) [2]

In order to manipulate the 6P growth the TiO_2(110) substrate surface has been rippled using ion beam bombardment. On the ion bombarded surfaces only island consisting of upright standing molecules are formed. The islands' length-to-width ratio can be adjusted by the ripple length. The islands exhibit compact rims and tend to terminate in the ripple valleys. (Fig 2) This is due to a detachment rate anisotropy caused by the position dependent binding strength [2]. The ripples actually represent highly stepped areas with alternating ascending and descending steps. Molecules attaching at the bottom terrace can bind with their full length whereas the binding length of those attaching from the upper terrace is reduced by the step height. Fig. 2 b.

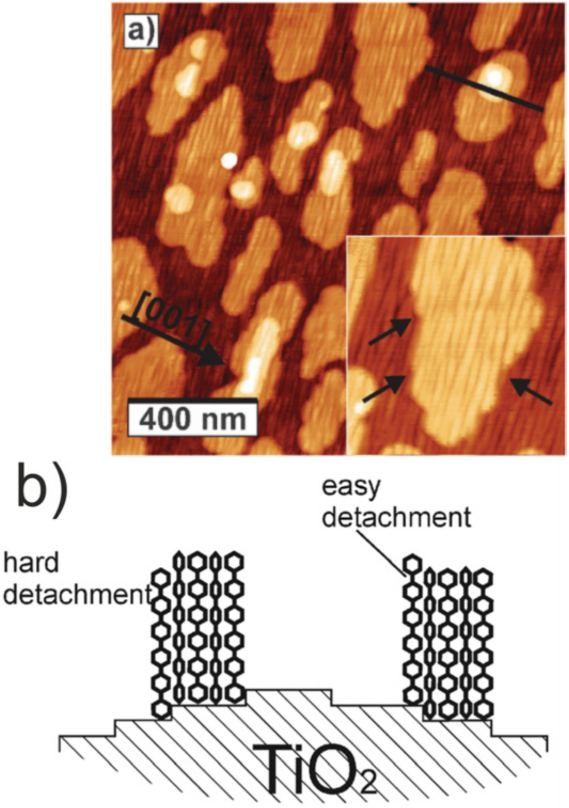

Figure 2: *a)AFM topography image of 6P islands with an average length to width ration of 4.5:1 on a highly rippled TiO_2 substrate. In the inset the discrete width and the straight compact island rims are well visible. b) illustration of reduced binding length due to the substrate step structure (From [2]).*

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Cooperation

F. Krok Institute of Physics, Jagiellonian University, Krakow, Poland (Ion bombardment, STM, nc-AFM)

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Surface Physics & Scanning Probe Microscopy

Organic Thin film growth on Graphene substrates

M. Kratzer, B. Kaufmann, C. Teichert
Markus.Kratzer@unileoben.ac.at

One promising application of graphene (Gr) is to use it as transparent, mechanically flexible electrode in organic electronics. The close relation between the hexagonal structure of graphene's basal plane and the aromatic backbones of many organic semiconductor molecules promises a high graphene-organic molecule interface quality. In order to fabricate organic devices with Gr electrodes, it is essential to understand the basics of organic thin film growth on Gr.

Here, we use the rod-like molecules para-hexaphenyl (6P) as a model representative for non-polar and dihydrotetraazapentacene (DHTAP) as representative of polar small organic molecules to investigate the growth of organic thin films on graphene. Such investigations using 6P have already been performed on exfoliated Gr on SiO_2/Si as "ideal" Gr model substrate. [1,2]

However, the technologically relevant fabrication of graphene is by chemical vapor deposition (CVD). Typically, Gr is grown on a copper catalyst which is then removed. During catalyst removal and transfer, the Gr is stabilized by the help of a thin polymethylmethacrylate (PMMA) layer spin coated onto the Gr-Cu substrate prior to Cu etching. The CVD Gr is then transferred to any desired substrate and the PMMA layer is removed. However, a complete removal of the PMMA is quite challenging and often not completely accomplished. The influence of PMMA residuals and the applied cleaning procedures on the organic thin film morphology is vastly unknown. An effective method to reduce the amount of PMMA is annealing in hydrogen atmosphere. We investigated the morphological changes of 6P thin films on CVD graphene PMMA transferred to SiO_2 as a function of the hydrogen annealing temperature. [3] The results are compiled in Fig. 1. With increasing annealing temperature the amount of PMMA residue reduces (Fig 1 a), however this is also accompanied with a degradation of the Gr as confirmed by Raman measurements (Fig 1 b).

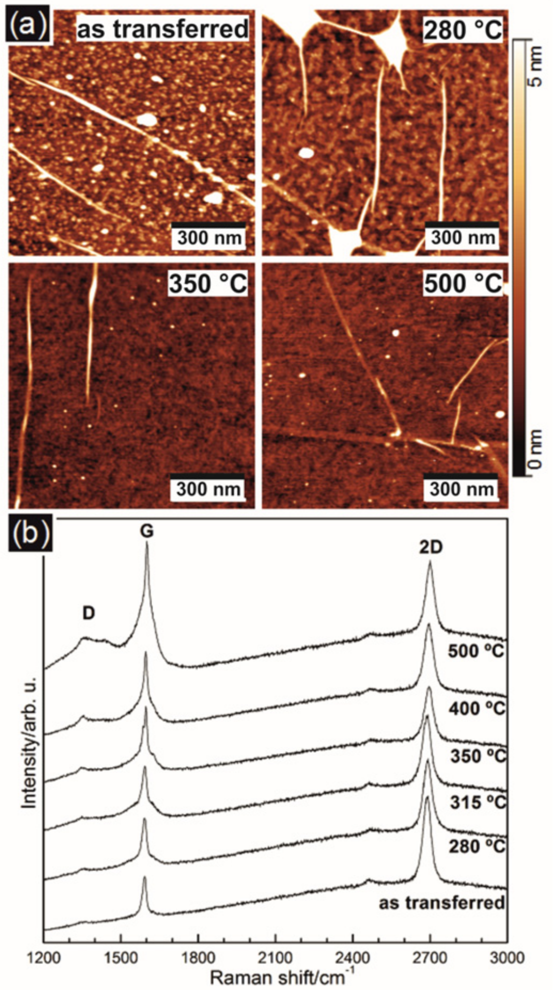

Figure 1: *a) AFM topography images of the PMMA transferred CVD graphene subjected to hydrogen annealing at different temperatures. b) Corresponding changes in the Raman spectra due to hydrogen annealing (from[3]).*

Sub monolayer 6P deposition at 90°C results in needle like structures consisting of molecules with their long axes oriented parallel to the substrate surface (Fig 2 a,b). On the as transferred Gr substrate the needles grow short since they avoid PMMA (Fig 2a). They can just extend in the PMMA free areas. With reducing PMMA residues more space is available and the needles grow longer (Fig 2b, c). Apparently the 6P-Gr interfacing is rather robust against contamination and damage, which is an advantage for device fabrication since this implies that extensive time consuming and costly Gr cleaning might not be necessary for all applications.

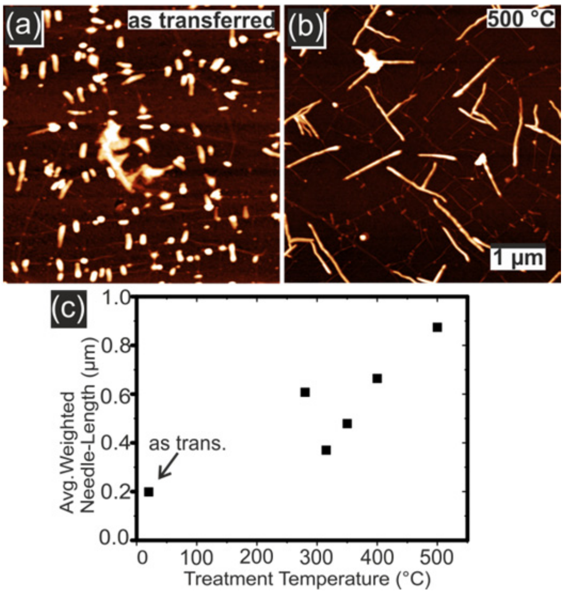

***Figure 2:** AFM topography images of 6P on as transferred CVD Gr (a) and on CVD graphene after 500°C hydrogen annealing (b). c) Average weighted 6P needle length as a function of hydrogen annealing temperature(from [3]).*

In contrast to 6P, DHTAP is a polar molecule carrying a permanent dipole moment. The dipole interaction leads to higher binding energies between the molecules which can result in more stable bulk properties. We investigated the growth morphologies of DHTAP on micro-mechanically exfoliated Gr supported by SiO_2/Si substrate. Against CVD Gr, this sort of Gr is easier to fabricate and, therefore, often favored in fundamental research. It was found that the growth morphologies of DHTAP strongly depend on the substrate temperature T during the deposition process. For lower T, the molecules form small elongated disorganized islands. For higher T, the molecules build curved oriented needle like structures.

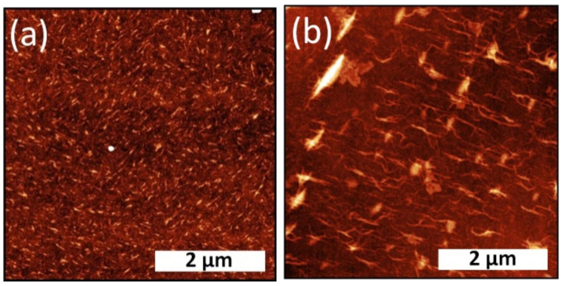

***Figure 3:** AFM topography images of DHTAP on exfoliated Gr. The substrate temperature during deposition was room temperature (a) and 80°C (b).*

Funding

- ÖAD Project Fr 17/2013 (Jan. 2013-March 2015)
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Cooperation

- B.C. Bayer: Faculty of Physics, University of Vienna, Vienna, Austria
- S. Hofmann: Department of Electrical Engineering, University of Cambridge, Cambridge, UK
- Conrad Becker; CiNaM, Marseille, France

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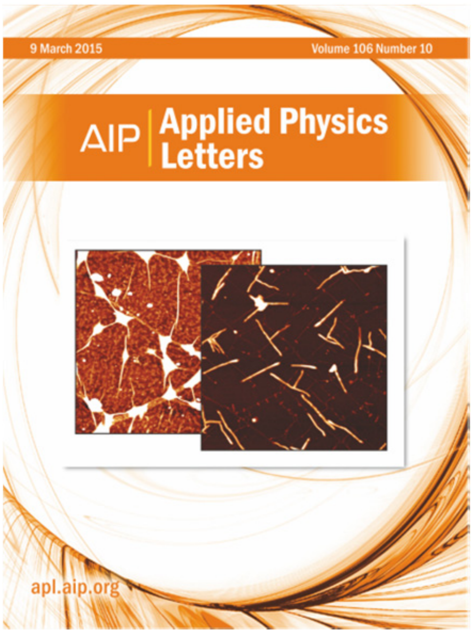


The authors were invited to design the cover art of the corresponding issue of Appl. Phys. Lett.

Surface Physics & Scanning Probe Microscopy

Piezoresponse force microscopy to determine the domain orientation distribution function of PZT materials.

M. Kratzer, M. Lasnik, C. Teichert
Markus.Kratzer@unileoben.ac.at

Here, piezoresponse force microscopy (PFM) was used to determine the domain orientation distribution function (ODF) of PZT (Lead zirconate titanate) materials. PFM is an atomic force microscopy based method that allows the measurement of the local piezoresponse. For that, a conductive AFM probe is scanned in contact mode over the surface while an alternating voltage is applied to the probe tip. The high electric field at the tip apex induces electrostrictive deformation of the material under the tip. The small movements of the surface are transferred to the AFM probe and can be read out via the optical AFM feedback using a lock-in technique. Vertical response is determined via the cantilever deflection and lateral response is read out via the cantilever torsion. Measuring the vertical response together with the lateral response in two independent directions (also called vector PFM) allows a reconstruction of the polarization orientation of the domains. A program based on the commercially available software Mathematica was developed to automatically evaluate vector PFM data and to reconstruct the ODF. In Fig. 1 the resulting ODF and domain orientation map of a unpoled PZT sample is shown. In Fig. 1a) the lock-in x-signal for the vertical response of the unpoled sample is shown. In Figure 1b) the reconstructed domain orientations are presented by a color code reflecting the azimuthal angle φ and polar angle θ.

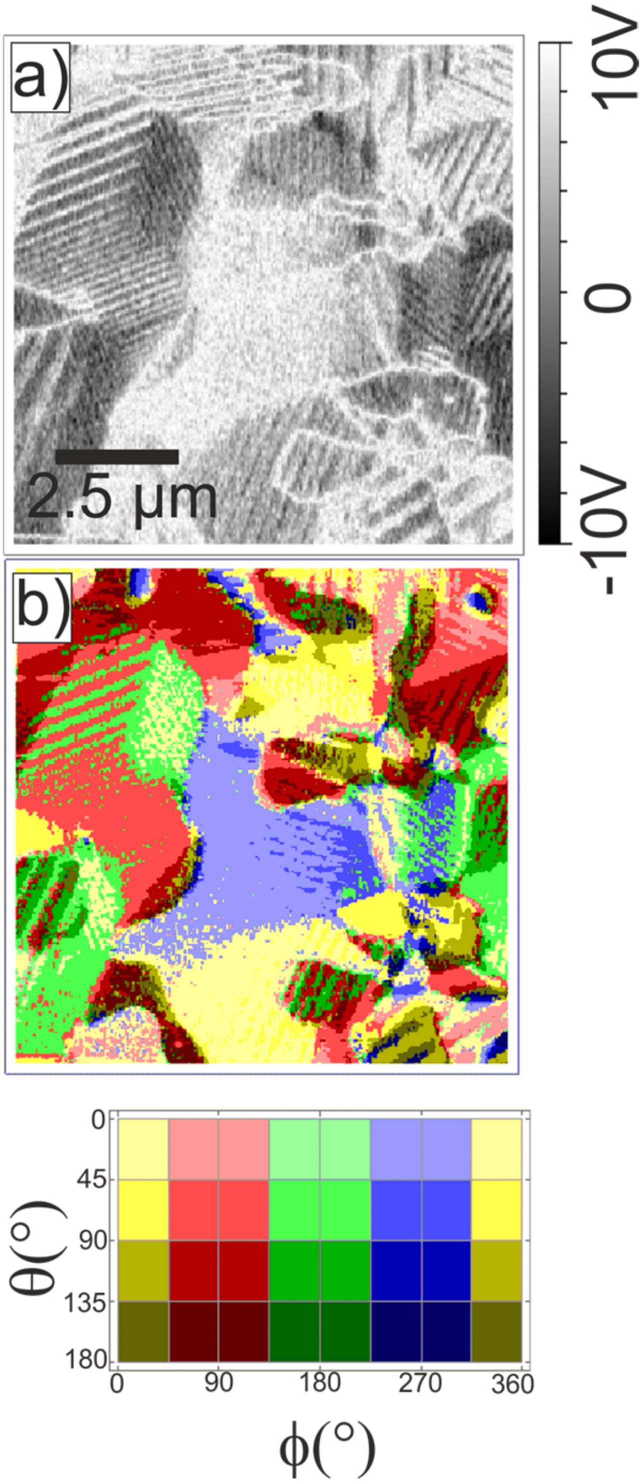


***Figure 1**: a) PFM (lock-in x)-signal of an unpoled PZT sample. b) Reconstructed domain orientation map.*

Funding

FWF Project # TRP 302-N20 “Bridging length scales in piezoceramics for commercial actuators”

Cooperation

- Dr. M. Deluca, MCL Leoben, Austria
- Dr. S. Röhrig and Dr. P. Supancic, ISFK MU Leoben

Surface Physics & Scanning Probe Microscopy

Morphology evolution of solid oxide full cell electrodes under long-term degradation

Patrice Kreiml, Christian Ganser, Kevin Gradwohl, Christian Teichert
teichert@unileoben.ac.at

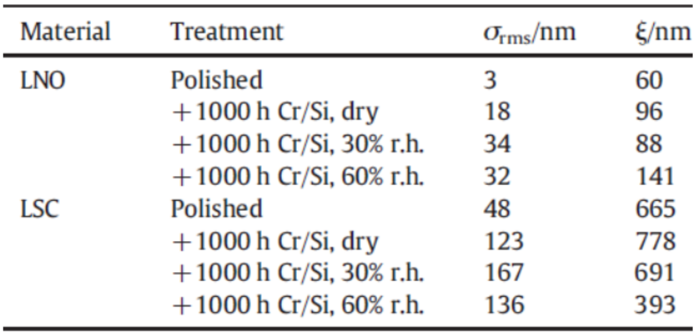
Solid oxide fuel cells (SOFCs) are high-temperature devices which enable highly-efficient and low-noise conversion of chemical to electrical energy. Although the SOFC technology has reached a high level of maturity with respect to performance and efficiency, long-term degradation remains one of the main technical challenges. Many degradation phenomena take place at the cathode and its interface to the electrolyte. A well-known mode of degradation is chromium poisoning of the cathode by gas phase transport of volatile Cr-species released from metallic interconnects.

In collaboration with the Chair of Physical Chemistry, the surface morphology of intermediate temperature SOFC cathodes were investigated. In this study the long-term stability of two promising cathode materials $La_{0.6}Sr_{0.4}CoO_{3-\delta}$ (LSC) and $La_2NiO_{4+\delta}$ (LNO) in dry and humid atmosphere at 700 °C were examined. For subsequent periods of 1000 hours up to a total time of 4000 hours the sample morphology was investigated by atomic force microscopy (AFM) as presented for the case of LSC in Fig. 1.

1) Roughness evolution

The AFM images were analyzed in terms of the root mean square (rms) roughness σ and the lateral correlation length ξ. The AFM measurements showed an increase in roughness over time. For both cathode materials, the highest rms-roughness was recorded after 3000 hours (see Tab. 1).

Tab. 1 *rms roughness σ and lateral correlation length ξ of LNO and LSC samples, determined at different stages of the degradation experiments. (From [1].)*



Material	Treatment	σ_{rms}/nm	ξ/nm
LNO	Polished	3	60
	+1000 h Cr/Si, dry	18	96
	+1000 h Cr/Si, 30% r.h.	34	88
	+1000 h Cr/Si, 60% r.h.	32	141
LSC	Polished	48	665
	+1000 h Cr/Si, dry	123	778
	+1000 h Cr/Si, 30% r.h.	167	691
	+1000 h Cr/Si, 60% r.h.	136	393

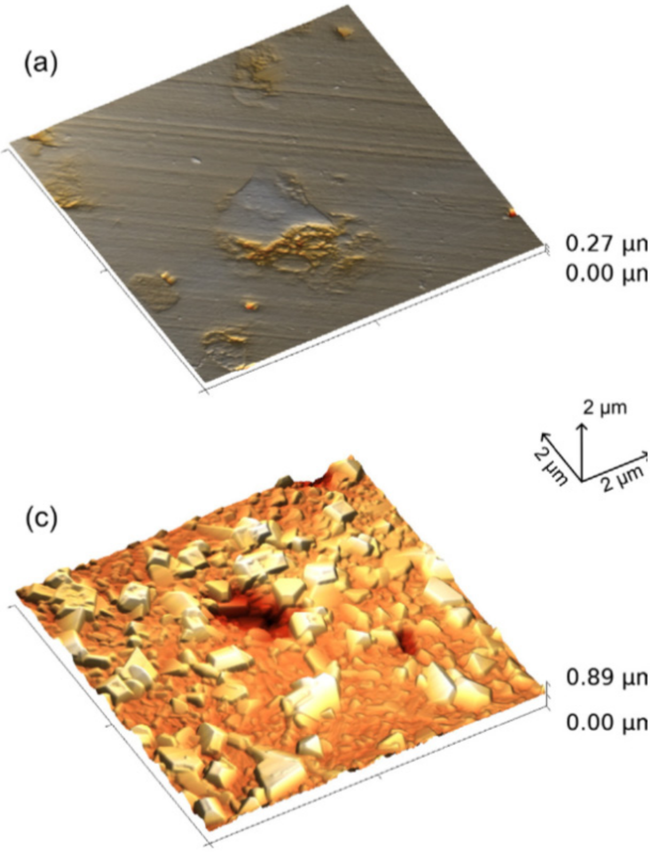


Figure 1 *10 µm × 10 µm AFM scans in three-dimensional illuminated presentation of (a) the fresh, polished LSC surface and (c) after an 2000 h of exposure to a Cr- and Si-source in a moderately humidified atmosphere (30% r.h.) (From [1].)*

2) Facet formation

For both samples, the formation of facetted crystallites is the main reason for the increase in σ as can be seen already in Fig. 1 c). By means of high-resolution AFM images, the three-dimensional shape of some of these crystallites could be revealed (see Fig. 2). These images allowed to determine the relative angles between the individual facets. By assuming the formation of strontium chromate ($SrCrO_4$) crystallites with monazite-type monoclinic structure as revealed by transmission electron microscopy [2], we could index the individual facets as presented in Fig. 2b).

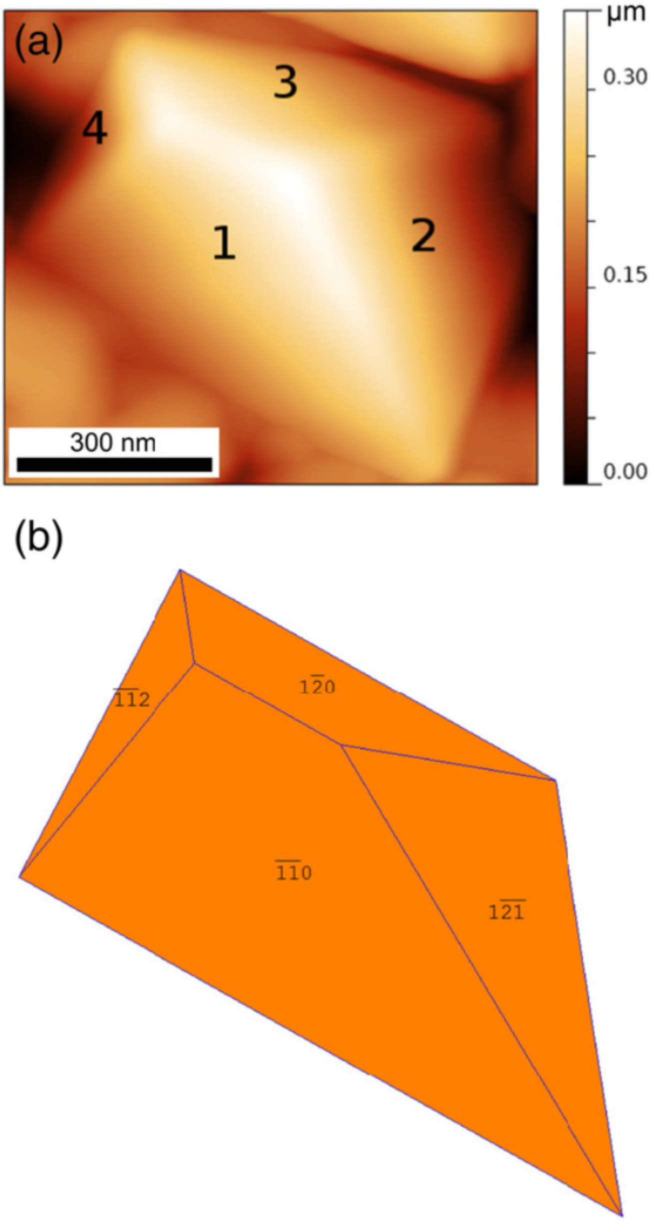


Figure 2: *(a) High-resolution AFM image of a SrCrO4 crystal on the surface of degraded LSC and (b) model of a $SrCrO_4$ single crystal with indexed faces (From [2].)*

Cooperation

- Edith Bucher, Nina Schrödl, Andreas Egger, Werner Sitte, Chair of Physical Chemistry, Montanuniversität Leoben;
- Christian Gspan, Ferdinand Hofer, Institute for Electron Microscopy and Nanoanalysis (FELMI), Graz University of Technology and Graz Centre for Electron Microscopy, Graz.

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Photonic Simulation for Electronics and Mining

The two projects described in this report are a continuation of work which started with experimental and numerical studies of ceramic photonic crystals (PhC) for microwaves and millimeter waves. Further developments concerned the inclusion of disorder, and PhCs made from semiconducting materials. The work reported in section 2 is an extension to a frequency several orders of magnitude higher – the extreme ultraviolet – with relation to nanolithography. A further development for strongly disordered solids concerned the two-dimensional modelling of the microwave absorption in heterogeneous rocks. Section 1 describes the extension to a three-dimensional model for a two-component hard rock.

1) 3D modelling of microwave absorption in heterogeneous solids with application in mining

Ronald Meisels, Michael Toifl
meisels@unileoben.ac.at

Motivation.

In mining fragmenting rocks requires a substantial expenditure of energy [1]. Most of this energy is not intrinsically required as the energy to form new surfaces but is lost as heat [2]. To reduce the power required, the internal structure of the rocks can be weakened by the production of damage. This is achieved applying microwaves propagating into the rocks and producing stress

Methods of simulation

To simulate the propagation of microwave radiation in rocks the finite difference time domain (FDTD) method [3] is used. The FDTD method discretizes the Maxwell equations. From the spatial distribution of the electric field the change of the magnetic field from one time step to the next (and vice versa) is determined.

The fields have to be stored in memory. To achieve the necessary resolution for the simulation, and fast parallel computation the calculations were performed at the EVA computation cluster at the Montanuniversität Leoben.

Model

A realistic model of the grain structure is constructed by dividing the rock into a large number of irregular polyhedra. Each polyhedron is randomly assigned to a phase, e.g., quartz or plagioclase, with the corresponding dielectric properties. The polyhedra are determined by a Voronoi tessellation. Points, called "seed points" are randomly distributed through the rock structure. To each seed point the set of all points closer to this point than to all others forms one of the polyhedra. The microstructure (brown in Fig. 1 center and right) is most relevant close to the center of the structure near the rock-air interface where the simulated microwaves from the source are incident. To avoid excessive computation times and memory requirements while having sufficient resolution in this relevant region the rest is simulated by a homogeneous model. Further out, the PML boundary condition is used to omit unphysical reflections at the limit of the computational domain.

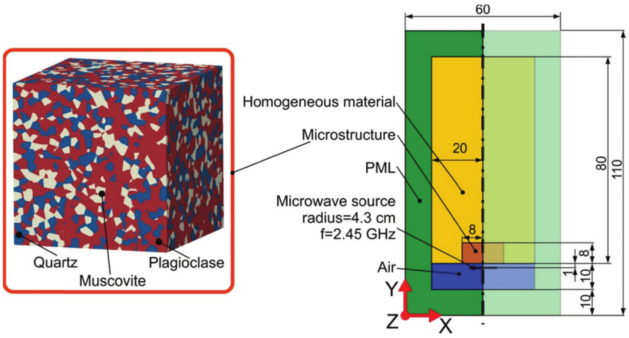

Figure 1 *Left: Two-phase model of the inhomogeneous rock structure (blue: e.g. quartz phase, white: e.g. plagioclase phase. Right: embedding of the micro structure in a homogeneous-model region (yellow).*

In the FDTD calculation program for each grid point the real part of the local dielectric constant and the conductivity has to be supplied by a function to simulate the Maxwell equation

$$rotH = \frac{\partial}{\partial t}D + j = \frac{\partial}{\partial t}\kappa'\epsilon_0 + \sigma E.$$

here κ' is the real part of the dielectric constant and the conductivity σ is related to the imaginary part of the dielectric constant κ'' via the relation $\kappa'' = \sigma/\omega\epsilon_0$.

A fast search tree algorithm quickly determines for each grid point to which polyhedron it belongs and what the local κ' and σ is.

The microwave source is simulated by introducing additional currents which generate a Gaussian beam. With this input, the electric field distribution is calculated. The squared electric field E^2 (shown in Fig. 2) is used to determine the heat generated by the absorbed power density $p = \sigma E^2$ due to Joule heat (shown in Fig. 3). The results of the electromagnetic simulation are used to determine the heat input for a thermal FEM (finite element method) simulation determining the temperature distribution in the rock. Fig. 4 shows this temperature distribution for 25 kW pulses of different durations. These temperature distributions, in turn, are used by another FEM calculation to determine the internal stresses within the rock. Fig. 5 displays the distribution of the maximal principal stress component. In this way it is possible to determine where the stress exceeds the limits of the rock and where the desired cracks are formed.

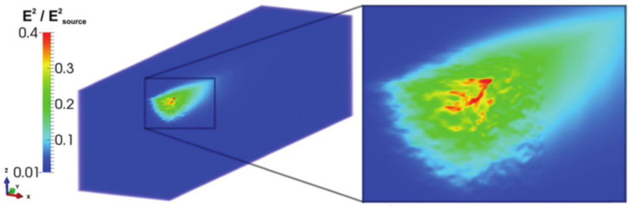

Figure 2: *Distribution of the squared electric field* E^2 *as determined by a FDTD calculation shown for the central inhomogeneous region modelled as in Fig 1 left. Shown is a quarter of the total volume. Irradiation is in the positive y direction.*

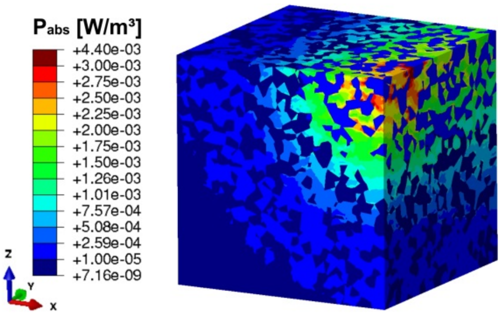

Figure 3*: Absorbed power density* p_{abs} *determined from the field distribution as shown in Fig. 2.*

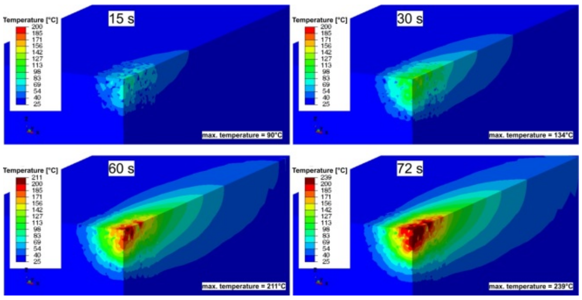

Figure 4: *Calculated temperature distribution for different durations of a 25 kW microwave pulse.*

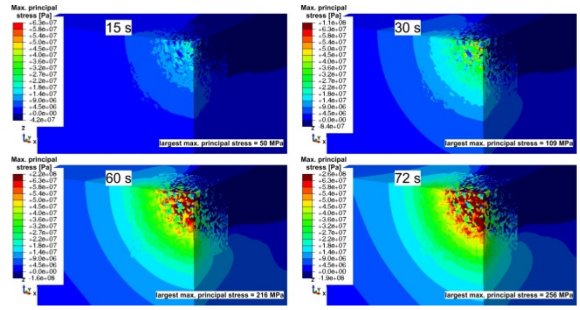

Figure 5: *Resulting maximal principal stress for the different durations of a 25 kW microwave pulse.*

Funding

The work was supported by the Austrian Science Fund (FWF) project TRP 284-N30.

Cooperation

This work was performed in a collaboration of the Institute of Physics (R. Meisels, F. Kuchar), the Institute of Mechanics (M. Toifl, T. Antretter) and the Chair of Mining Engineering and Mineral Economics (P. Hartlieb) at the Montanuniversität Leoben.

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2) Photonic Structures as Mirrors for Extreme Ultraviolet (EUV) Lithography

Ronald Meisels, Friedemar Kuchar
meisels@unileoben.ac.at, kuchar@unileoben.ac.at

Motivation

In microelectronics, at present, 193 nm UV radiation is used to produce structures of ever increasingly finer resolution. To further reduce the dimensions of the electronic components, especially the transistors, a transition to EUV radiation is a promising option. A proposed source for 13.5 nm radiation [6] is a Sn plasma produced by laser pulses. In this wavelength range ordinary metallic mirrors cannot be used since the dielectric constant is no longer strongly negative, but close to unity. Here Bragg reflectors consisting of multiple layers are used to increase the reflectivity by constructive interference.

In this work, the influence of different design parameters on the reflectivity is studied.

Method

To calculate the reflectivity of an array of different plane parallel layers the multiple scattering method (MSM) [4,5] is used. The scattering of each layer can be described by a scattering matrix **S** which transforms the incident wave amplitudes into the outgoing wave amplitudes. The diagonal matrix elements correspond to the reflection coefficients, the off diagonal components to the transmission coefficients. From this matrix the transfer matrix **M** is calculated which converts incident and outgoing amplitudes on one side of the layer to those on the other side. The advantage of this matrix is that the transfer matrix of a structure consisting of many layers is determined as the matrix product of the transfer matrices of the individual layers. Reflectivity and transitivity of the whole multilayer structure is found by transforming the product matrix back into a scattering matrix. The program MULTEM presented in Refs. 4 and 5 determines reflectivity and transmission in this way. In addition to homogenous layers regular two-dimensional arrays of spheres of one material embedding in another can be studied.

To study more complex structures the FDTD method has to be used. By using a pulsed wave the properties of the structure in a range of frequencies can be studied.

Result: Choice of materials

Near 13.5 nm Si has a dielectric constant ε with a real part close to 1 and a small imaginary part. The peak reflectivity of structures of 40 double layers consisting of Si and a material with complex dielectric constant ε in the range of $0.75 < \mathrm{Re}(\varepsilon) < 0.95$ and for $\mathrm{Im}(\varepsilon) < 0.12$ was calculated and is shown in Fig. 6. For ε close to unity the EUV radiation propagates deeply through the layers. This transmission reduces the reflectivity. To avoid this effect the calculation is repeated for 4096 layers (bottom diagram of Fig. 6). In this design the optimal elements are found to be Mo and Nb.

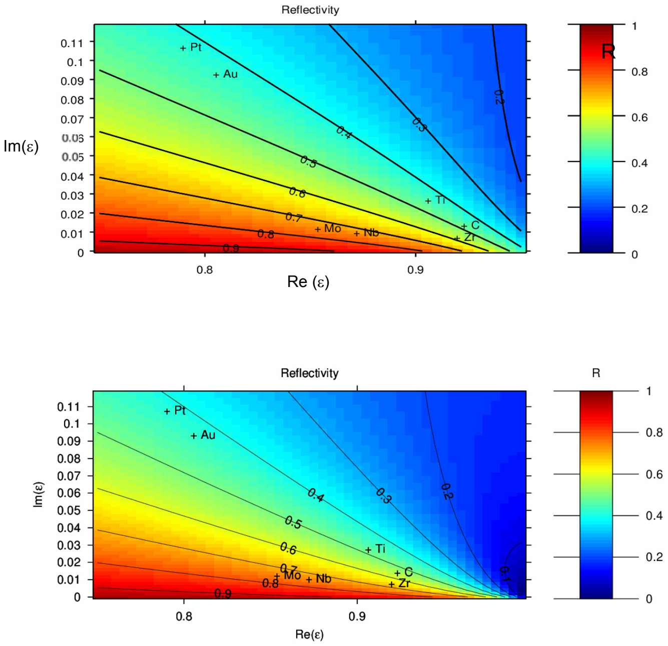

***Figure 6**: Dependence of the Reflectivity of 40 (top) and 4096 (bottom) double layers of Si and a material with complex dielectric constant ε. Marked with crosses are the values for various elements of technological interest at a wavelength of 13.5 nm.*

Result: 3D PhC structure of spheres

The MULTEM program is used to calculate the reflectivity of Mo spheres arranged in a bcc lattice which are embedded in a Si matrix (see Fig. 7) and in a hypothetical lossless (shown in Fig. 8) material, resp. .

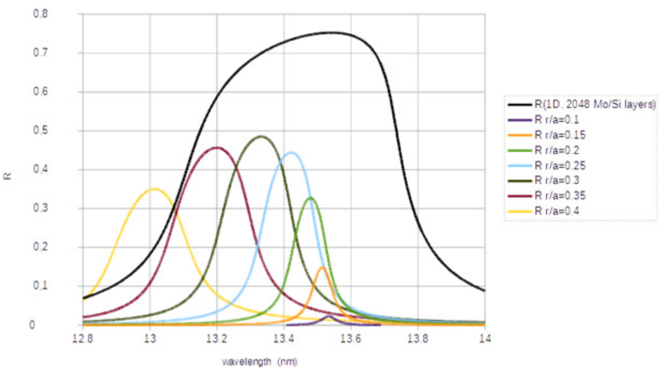

***Figure 7:** Reflectivity of a bcc lattice (cubic lattice constant a) of Mo spheres (radius r) ε=0.853+0.012i embedded in Si.*

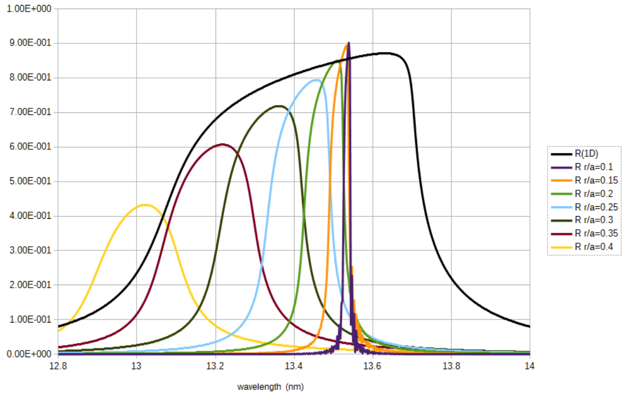

***Figure 8**: Reflectivity of a bcc lattice (cubic lattice constant a) of Mo spheres (radius r) $\varepsilon=0.8+0.03i$ embedded in vacuum ($\varepsilon=1$).*

Result: Complex 3D PhC "fishnet" structure

To calculate more complex structures the FDTD method has to be employed. To determine the reflectivity over a frequency range Δf the incident wave has to be a pulse (width $\Delta t \propto 1/\Delta f$) in the time domain and a plane wave in space. The time dependent field of the reflected wave is then Fourier transformed. In addition, the same wave is sent through an empty model to record the original incident field, which is Fourier transformed as well. The reflectivity is obtained as the squared ratio of the transformed reflected field relative to the transformed incident field.

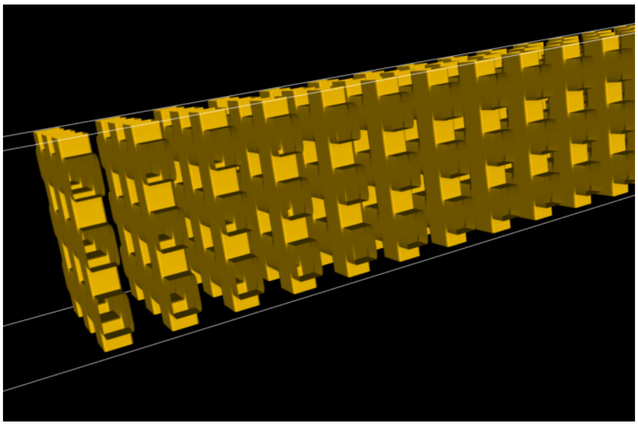

***Figure 9:** Photonic crystal with a so-called fishnet structure [7].*

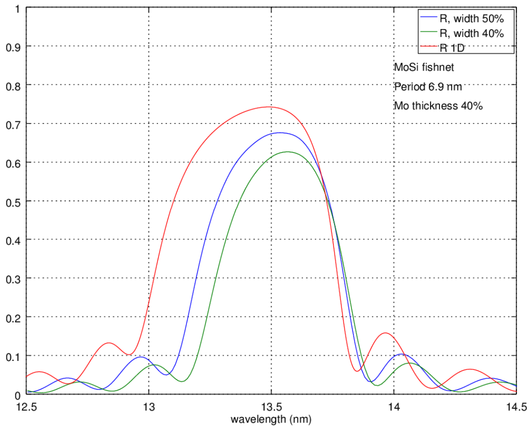

***Figure 10:** Reflectivity of the fishnet structure for a width of the fishnet beams of 40% and 50% of the lattice constant. The thickness of the fishnet layers is 40% of the period. The periodicity within each layer as well as of the layer sequence is 6.9 nm. For comparison the reflectivity of the 1D layer structure (40% Mo) is included.*

As an example, the fishnet structure shown in Fig. 9 was studied. The reflectivity for two realizations is shown in Fig. 10.

Conclusions

More complex PhCs than the 1D layer structure are explored. Among the elements, in addition to the presently used Mo, Nb is found to yield similar peak reflectivities in 1D layer structures. A 3D PhC made of Mo spheres embedded in a vacuum (or air) yield higher peak reflectivities than the 1D structure, but with a narrow bandwidth (narrower than the Sn plasma emission) which is a disadvantage concerning EUV lithography. On the other hand, the narrow band width could be useful for applications as filters.

Further investigations will study other complex structures using the FDTD method.

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Simulation of Quantum Electron Transport

Manifestation of Many-Particle Physics in the Integer Quantum Hall Regime

Josef Oswald
josef.oswald@unileoben.ac.at

While the fractional quantum Hall effect (FQHE) is understood in terms of quasi particles (Composite Fermions) in the highly correlated many-particle electron system, it is widely believed that the physics of the integer quantum Hall effect (IQHE) is dominated by interacting single electrons. The type of interaction plays an important role for the screeing behavior of the electron system. Up to date the widely accepted model for screeing in the IQHE regime has been developed by Chlovskii, Shklovskii and Glatzman (CSG), who addressed the electrostatics of the edge channel region [1]. Their key ingredient is the different screeing behavior of partly and fully filled Landau Levels (LL) and instead of getting narrow quasi one-dimensional channels they get stripes of partly filled LLs that can get up to hundreds of nanometers wide. These stripes of partly filled LLs are known as the so called compressible stripes, that get separated by usually narrow incompressible stripes of fully filled LLs. The main result of CSG is that the screening property of the compressible stripes screens out almost the entire slope of the edge potential near the sample boundaries and generates terraces in the uprising edge potential. At the same time the electron density and the local filling factor changes continuously across the compressible stripes.

There are two main reasons for our motivation to reconsider this problem on the basis of a more general many-particle approach. The one is that it is well known and also widely accepted that there exists an enhanced g-factor for spin splitting that is driven by exchange interaction, which is exclusively a many particle effect. The other reason is based on recent scanning gate (SG) experiments by the Ensslin group at the ETH Zürich who investigated edge stripes passing quantum point contacts (QPC) at high magnetic field [2]. Their analysis of the data indicates that the screening behavior within the compressible stripes appears to be much weaker than predicted by models based on CSG. The CSG approach is based on classical electrostatics and therefore many particly physics, especially exchange effects, cannot be introduced in this approach. The only that can be done with the CSG model is to introduce the exchange enhanced g-factor as a semi-empirical parameter by hand, which might not be sufficient to capture all relevant many-particle effects.

In order to reconsider the whole problem, we need on the one hand a modeling for the many-particle groundstate; on the other hand we need a model for electron transport close to equilibrium while driving the electron system out of equilibrium. At the same time the transport model must not make use of single electron flow like in semi classical models. We have shown that the non-equilibrium network model (NNM) [3], that we developed further over many years, is able to meet these requirements [4]. We also adapted a numerical Hartree-Fock model [5] for exchanging data with the NNM and as a first application we demonstrated that SGM experiments have the potential for imaging condensed localized quantum states [6].

Our simulations so far have used the Coulomb interaction (Hartree potential). However, exchange effects have no local representation and therefore cannot be transferred to the NNM by any local screened potential. Instead, the carrier distribution and the local filling factor capture both, the Hartree and the exchange effects and in Ref.4 we have shown, that the NNM can be used in two versions, a Hartree version and a filling factor version, that turns out to be more suitable for many-particle electron systems.

In the following we give some examples for typical results that can be obtained by the improvements that we achieved in the last two years.

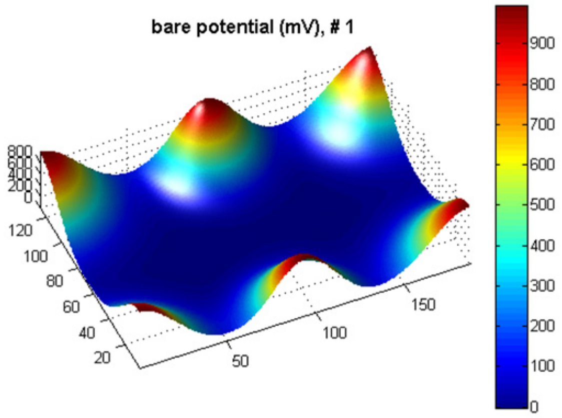

Figure 1: *Bare potential for a Hall bar of size 600x400nm with edge potential and voltage probes as used for the Hartree-Fock calculations below. The edge potential is created by repulsive Gaussian peaks of 1000mV amplitude that leave openings for current contacts at the ends and voltage probes along the sample. The x and y- directions are labelled in gridpoint numbers of the NNM. A random disorder potential with amplitude of approximatly ±10mV is generated by randomly distributing Gaussian peaks, which is not visible on the scale covering 1000mV.*

Fig.1 shows the bare potential of a Hall bar structure of total size of 600x400nm that gets filled with 480 electrons, which corresponds to an average carrier density of $n = 2x10^{11}cm^{-2}$. The solution of the Hartree-Fock model for different magnetic fields deliver arrays of the local filling factors separately for electrons with spin 1 and spin 2. That is transferred to the NNM which calculates the lateral distribution of the experimentally injected non-equilibrium electrochemical potentials. No local quantities like local conductivities or local Ohm's law is used up to this point, because that would imply the (forbidden) possibility to track down the path of the electrons while moving from one current contact to the next. Even the Landauer formula is not used up to this point for finding the selfconsistent solution for the chemical potentials. Only as a postprocessing step, after obtaining the solution, currents are calculated at the designated current contacts only and potential differences are taken from the voltage probes and from these, the associated resistances and conductances are calculated like done also in real experiments.

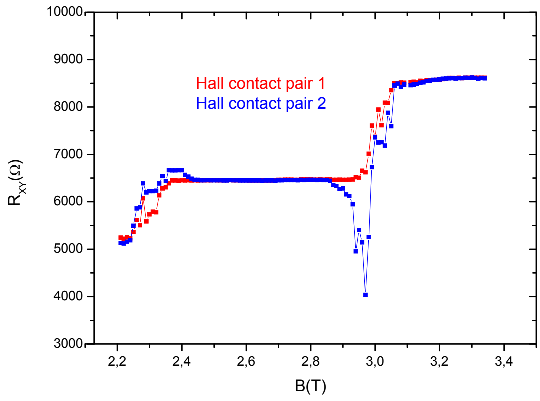

Figure 2: *Simulated Hall resistance as a function of magnetic field for the two Hall contact pairs.*

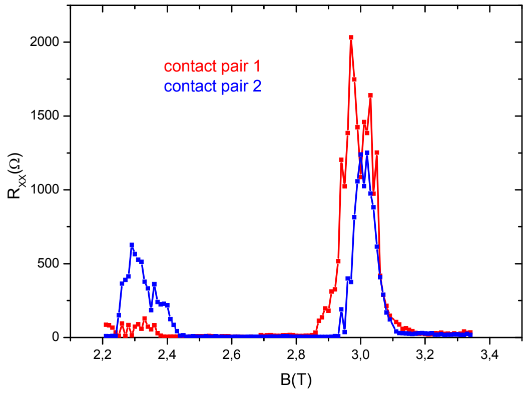

Figure 3*: Simulated longitudinal resistance as a function of magnetic field for the two longitudinal contact pairs.*

As can be seen from Fig.2 and Fig.3 the obtained Hall resistance and longitudinal resistance show the expected behavior and exhibit Hall plateaus at zero longitudinal resistance and R_{xx} peaks in the transition regime between QH plateaus. The average electron density of $2x10^{11}cm^{-2}$ of the 480 electrons corresponds to an effective density of about $2.5x10^{11}cm^{-2}$ in the active region of the "structured" Hall sample and therefore the peaks and plateau positions are correctly shifted up in magnetic field. There appear strong resistance fluctuations in both, the Hall and the longitudinal resistance as has to be expected for quantum Hall structures of mesoscopic size, like it is also known from experiments.

Figures 4-6 show the local fillingfactor of the top spin1 Landau level (LL) during the $\nu = 4 \rightarrow 3$ plateau transition. The spin 1 level is higher in energy than the spin 2 level and therefore depletion starts with the spin1 level that is initially at filling factor ν =2, while for spin2 we have also filling factor ν=2, which gives in total filling factor ν=4. At the beginning of the plateau transition at B=2.91 Tesla (see Fig.4) the initially completely filled spin 1 LL starts to break up in sub-sections of filling factor ν=2, while there appear also sections of filling factor ν=1, which gives an average filling factor between ν=4 and ν=3.

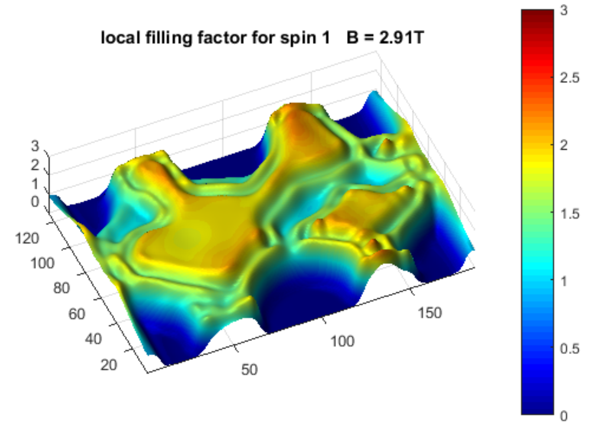

Figure 4*: Lateral filling factor distribution for the spin 1 electrons at the beginning of the $\nu = 4 \rightarrow 3$ plateau transition at B=2.91 Tesla. The colors represent the filling factor.*

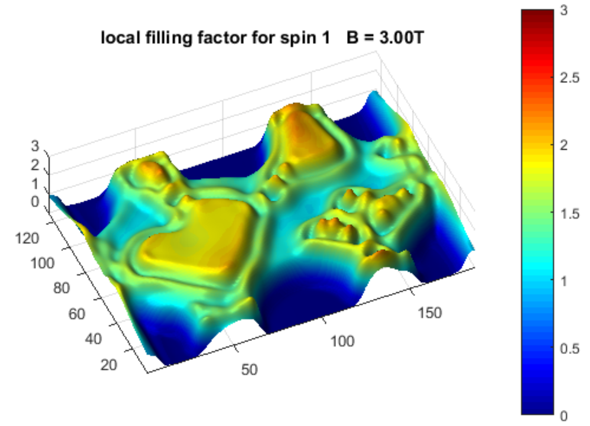

Figure 5*: Lateral filling factor distribution for the spin 1 electrons in the middle of the $\nu = 4 \rightarrow 3$ plateau transition at B=3.0 Tesla.*

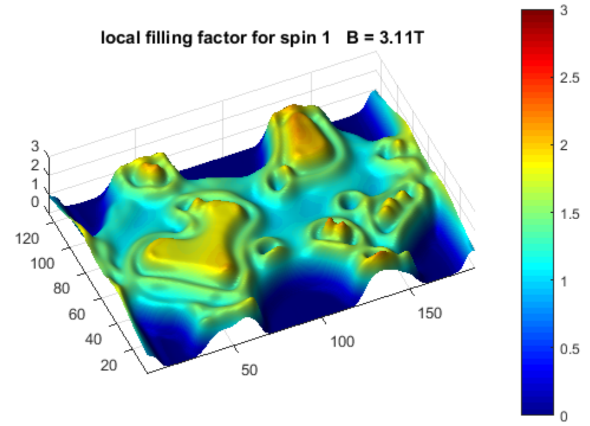

Figure 6*: Lateral filling factor distribution for the spin 1 electrons in the end of the $\nu = 4 \rightarrow 3$ plateau transition at B=3.11 Tesla.*

From Figs. 4-6 one can imagine how the de-population of the spin 1 LL works. Instead of getting an overall decrease of the carrier density, we get shrinking clusters of fully filled spin 1 LL at ν = 2 and increasing clusters of depleted spin 1 LL at ν = 1, which on average give a continuously decreasing filling factor. Therefore a total filling factor of ν = 1.5 is made up by half of the area taken up by clusters of filling factor ν=2 and half of the area taken up by clusters of filling factor ν=1. The same happens subsequently if the spin 2 LL gets de-populated, which stays at ν=2 while de-populating the top spin 1 LL. This is quite in constrast to the CSG model and is purely a result of many-particle quantum physics. But this can explain, why even a half filled LL provides only poor screening as compared to a Thomas-Fermi like behavior that allows a continuous carrier density variation all over the sample area. In addition, at the boundaries between clusters of filling factor ν=2 and ν=1 there appear terraces of almost constant filling factor ν=1.5 (see Figs. 4-6) which create transmitting channels in the NNM. Also this is in contrast to CSG who find transmitting compressible stripes of continuously varying carrier density. This behavior seems to result from a dendency of the many-particle system to avoid the appearance of partly filled spin 1 and spin 2 LLs at the same time. A similar behavior would result by applying Hund’s Rule, which seems to be the driving force for many particle effects like the exchange enhaced g-factor. In our modelling the exchange enhanced g-factor appears as a built-in effect without any need to introduce it by hand. The investigation of these finding is work in progress [7].

In Figs. 7-9 we finally show the lateral distribution of the non-equlibrium chemical potential for all three cases as shown in Figs. 4-6. If looking at the potential distribution for the different cases, one can see that the potentials are transmitted along the half-integer stripes appearing in the Figs. 4-6. If the potentials mix up at some locations this generates dissipation as it is the case in the transition regime of the IQHE. While this happens only weakly in Fig.7 and Fig.9, this mixing appears to be quite strong in Fig.8, which represents a case close to the maximum of the R_{xx}-peak.

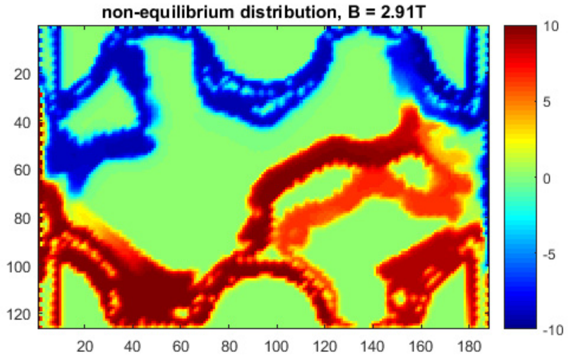

Figure 7: *Lateral distribution of the non-equilibrium chemical potential at the beginning of the ν = 4 → 3 plateau transition at B=2.91 Tesla. The colors represent potentials in arbitrary units.*

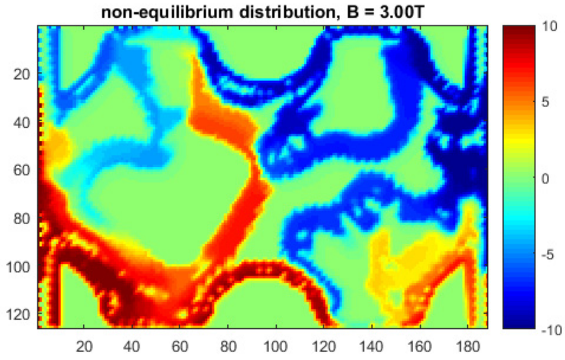

Figure 8: *Lateral distribution of the non-equilibrium chemical potential in the middle of the ν = 4 → 3 plateau transition at B=3.00 Tesla.*

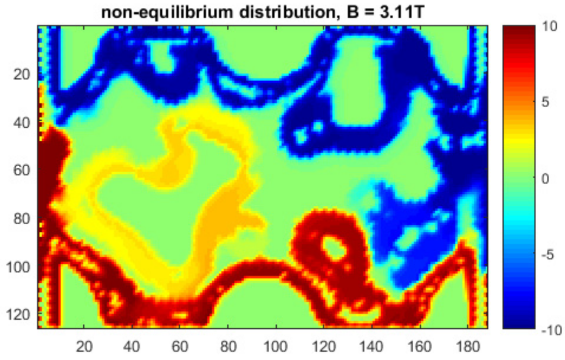

Figure 9: *Lateral distribution of the non-equilibrium chemical potential at the end of the ν = 4 → 3 plateau transition at B=3.11 Tesla.*

Cooperation

Rudolf A. Römer (University of Warwick, Department of Physics and Center for Scientific Computing, UK)

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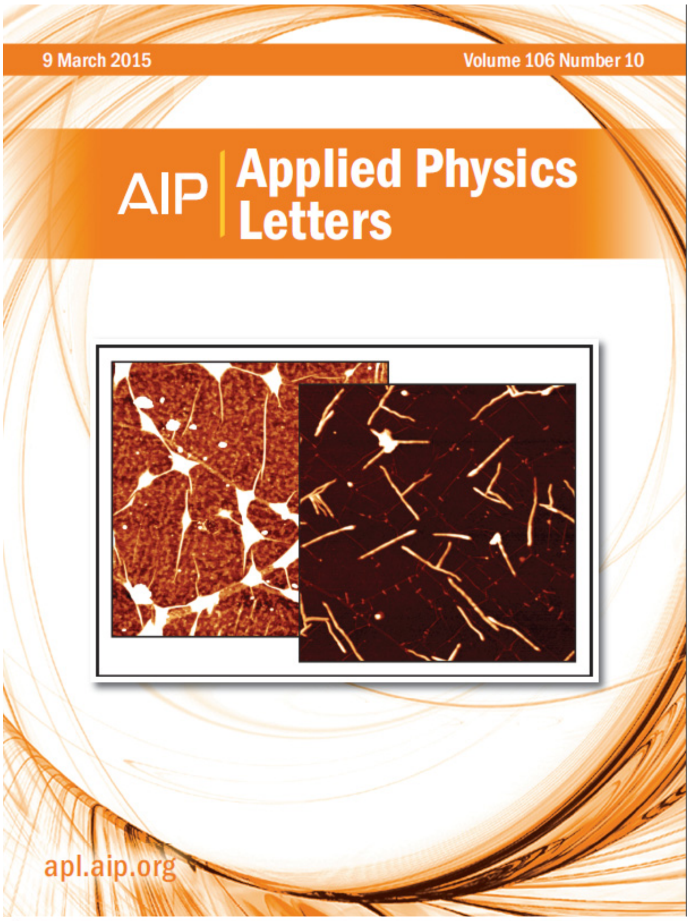
3.5 Cover pages in Journals and Books



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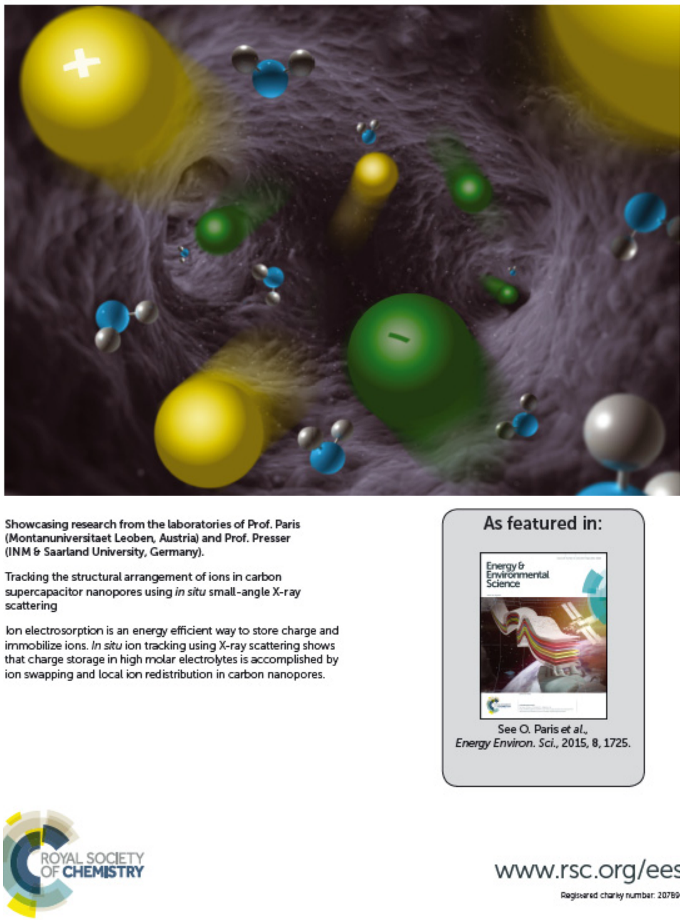

Showcasing research from the laboratories of Prof. Paris (Montanuniversitaet Leoben, Austria) and Prof. Presser (INM & Saarland University, Germany).

Tracking the structural arrangement of ions in carbon supercapacitor nanopores using *in situ* small-angle X-ray scattering

Ion electrosorption is an energy efficient way to store charge and immobilize ions. *In situ* ion tracking using X-ray scattering shows that charge storage in high molar electrolytes is accomplished by ion swapping and local ion redistribution in carbon nanopores.

As featured in:

Energy & Environmental Science

See O. Paris *et al.*, *Energy Environ. Sci.*, 2015, 8, 1725.

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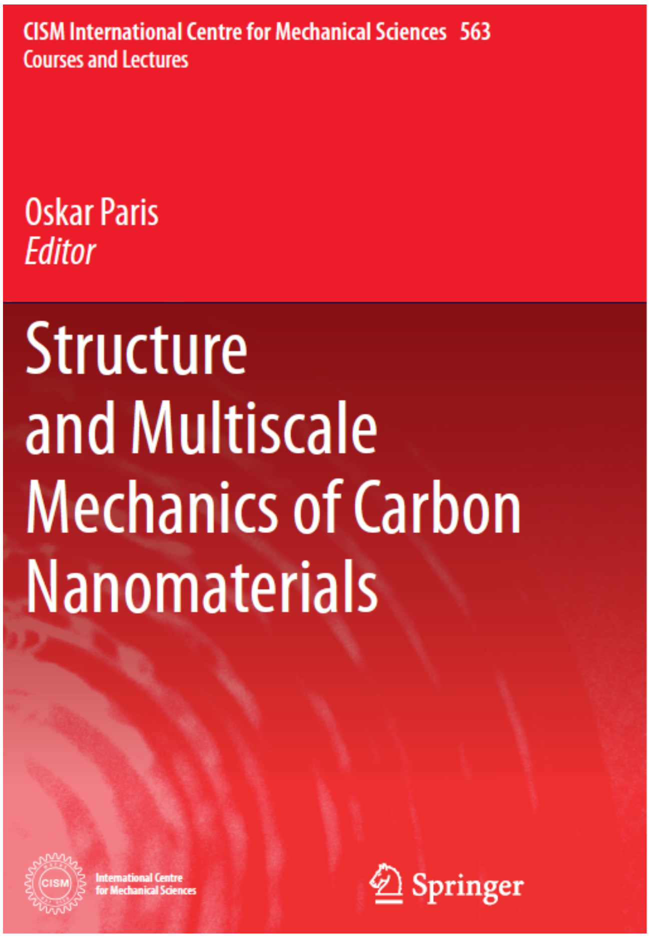


CISM International Centre for Mechanical Sciences 563
Courses and Lectures

Oskar Paris
Editor

Structure and Multiscale Mechanics of Carbon Nanomaterials

International Centre for Mechanical Sciences

Springer

4. Presentations

4.1 Talks at conferences

1. M. Burian, G. Fritz-Popovski, O. Paris and R.T. Lechner, Detailed shape retrieval of colloidal inorganic nanocrystals from SAXS-data, 64. Jahrestagung der Österreichischen Physikalischen Gesellschaft ÖPG 2014, Pöllau, Austria, 24.-27.9.2014
2. M. Burian, H. Amenitsch, G. Fritz-Popovski, M. Yarema, W. Heiss, M. Kovalenko, O. Paris, R.T. Lechner, In-situ Synchrotron Studies of Colloidal Crystallization and the Influence of the Nanocrystal Shape, Nanoscience with Nanocrystals NaNaX 6, Bad Hofgastein, Austria, 18.-23.5.2014
3. C. Ganser, F. Weber, U. Hirn, R. Schennach, C. Teichert, Characterization of cellulose materials by AFM based nanomechanical test, 4th Euro AFM Forum, Göttingen, Germany,17.-19.3.2014
4. M. Hartmann, Monte Carlo and Moleculardynamics Simulation Techniques, Advanced CISM course on Structure and Multiscale mechanics of carbon nanomaterials, Udine, Italy, 21.-25.7.2014 **(Invited)**
5. M.Hartmann, A simple model to study the influence of topology and distribution of reversible sacrificial bonds on the mechanical behavior of polymers, 64. Jahrestagung der Österreichischen Physikalischen Gesellschaft ÖPG 2014, Pöllau, Austria, 24.-27.9.2014
6. M. Kratzer, S. Klima, C. Teichert, Hexaphenyl thin films for tracking PMMA residuals on CVD grown graphene, 3rd Austrian Symposium on Carbon Based Coatings , Seggau, Austria 4.6.2014
7. M. Kratzer, C. Teichert, Growth morphologies of organic thin films on rippled TiO2 and CVD graphene substrates, 15th Joint Vacuum Conference, Vienna, Austria, 15.-20.6.2014
8. M. Kratzer, R. Wartbichler, C. Teichert, Organic thin film growth on rippled TiO2 and CVD graphene substrates, NanoSEA 2014, Marseille, France, 7.-11.7.2014
9. M. Kratzer, L. Kormos, P. Kreiml, E. Bucher, W. Sitte, C. Teichert, Atomic force microscopy based electrical and morphological investigations of La0.6Sr0.4CoO3-δ electrode surfaces, 14th International Metallography Conference 2014, Montanuniverisitaet Leoben, Austria, 17.-19.9.2014
10. M. Kratzer, Organic self assembled nanostructure growth on graphene substrates, 73 IUVSTA Workshop on “Nanostructures on two-dimensional solids, Eisenerz, Austria, 22-26.9.2014 **(Invited)**
11. F. Kuchar, B. Kramer, Zukünftige Tendenzen in der Halbleitertechnologie und der Computer gestützten Materialmodellierung, 60. Metallkundekolloquium, , Lech/Arlberg, Austria, 23.4.-25.4.3014 **(Invited)**
12. R. T. Lechner, R.T. Lechner, G. Fritz-Popovski, M. Yarema, W. Heiss, A. Hoell, T.U. Schülli, and O. Paris, Structural Profiles of Nanocrystals from ASAXS and Crystallographic Techniques, The 23rd Congress and General Assembly of the International Union of Crystallography (IUCr 2014), 8.-12.8.2014, Montreal, Kanada **(Invited)**
13. R.T. Lechner, G. Fritz-Popovski, M. Yarema, W. Heiss, and O. Paris, Metastable Crystal Phase in the Shell of PbS/CdS Core/Shell Nanocrystals, 64. Jahrestagung der ¨Osterreichischen Physikalischen Gesellschaft ÖPG 2014, , Pöllau, Austria, 24.-27.9.2014
14. R.T. Lechner, G. Fritz-Popovski, M. Yarema, W. Heiss, A. Hoell, T.U. Schülli, and O. Paris, Crystal Structure within the Shell of PbS/CdS Core/Shell Nanocrystals Influences the Photoluminescent Emission, Nanoscience with Nanocrystals NaNaX 6, Bad Hofgastein, Austria, 18-23.5. 2014
15. R.T. Lechner, M. Burian, C. Prehal, M. Yarema, H. Amenitsch, W. Heiss, and Oskar Paris, In-situ Synchrotron Studies of Colloidal Crystallisation and the Influence of the Nanocrystal Shape, DPG-Frühjahrstagung der Sektion Kondensierte Materie (SKM) 2014, Dresden, Germany, 30.3.-4.4.2014
16. S. Nabavi, M. J. Harrington, O. Paris, P. Fratzl, M.A. Hartmann, The influence of topology and thermal backbone fluctuations on sacrificial bonds, DPG Spring Meeting, Dresden-Germany, 30.3.-4.4.2014
17. S. Nabavi, M. J. Harrington, O. Paris, P. Fratzl, M.A. Hartmann “*Topology and thermal backbone fluctuations determine sacrificial bond efficacy*, Bio-inspired Materials, Potsdam, Germany,18.-21.3.2014
18. S. Nabavi, M.A. Hartmann “*The role of sacrificial bonding on the mechanical properties of polymer chains- a Monte Carlo study*”, 64. Jahrestagung der Österreichischen Physikalischen Gesellschaft ÖPG 2014, Pöllau, Austria, 24.-27.9.2014
19. O. Paris, Assessing structural hierarchy and mechanical behavior of nanostructured carbon materials, O. Paris, C. Prehal, H. Peterlik, V. Presser, XXIII International Materials Research Congress (IMRC), Cancun (MX) 18.08-21.08.2014. **(Invited)**

20. O. Paris, Water induced deformation of nanoporous materials , O. Paris, Hauptvortrag im Fachverband Metall- und Materialphysik, Frühjahrstagung des Arbeitskreises Festkörperphysik der deutschen physikalischen Gesellschaft 2013, Dresden (D) 30.03-04.04.2014. **(Invited)**
21. O. Paris, The zoo of carbon nanomaterials, CISM Advanced Course: Structure mand Multiscale Mechanics of Carbon Nanomaterials, Udine, 21-25 July, 2014. **(Invited)**
22. O. Paris, Structure and mechanical properties of carbon fibers, CISM Advanced Course: Structure and Multiscale Mechanics of Carbon Nanomaterials, Udine, 21-25 July, 2014. **(Invited)**
23. O. Paris, Highly porous carbons and plant derived carbons, CISM Advanced Course: Structure and Multiscale Mechanics of Carbon Nanomaterials, Udine, 21-25 July, 2014. **(Invited)**
24. C. Prehal, D. Weingarth, E. Perre, R. T. Lechner, H. Amenitsch, V. Presser and O. Paris, In-situ SAXS/WAXS as a Novel Method to Study Ion Transport in Nanoporous Systems at the Symposium on Ion Dynamics in Confined Systems, University of Cambridge 07/2014
25. C. Prehal, D. Weingarth, E. Perre, R. T. Lechner, H. Amenitsch, V. Presser and O. Paris, Ion transport phenomena in confined geometry studied by in-situ X-ray methods at 64. Jahrestagung der Österreichischen Physikalischen Gesellschaft ÖPG 2014, Pöllau, Austria, 24.-27.9.2014
26. C. Teichert, Probing cleanliness of graphene with small organic molecules, Energy Materials Nanotechnology Summer Meeting, Cancun, Mexico, 9.-12.6.2014 **(Invited)**
27. C. Teichert, Surface Science differently: What holds paper fibers together, Surface Science Seminar 3S'14, St. Christoph am Arlberg, 9.-15.3.2014
28. G. Fritz-Popovski, Moisture driven actuation of silica structures replicated from pine cone scales DPG Frühjahrstagung (18 March 2015)
29. R.T. Lechner, Nanoparticles and Nanopores for Energy Applications: Scattering/Diffraction and Microscopy, 1st CERIC New Users Symposium for multi-technique research at the new SOLARIS Synchrotron, 24.6.-25.6. 2015, Krakow, Poland **(Invited)**
30. R.T. Lechner, M. Burian, H. Amenitsch, C. Karner, M. Yarema, W. Heiss, C. Delago and O. Paris, Dynamics of Colloidal Crystallization and the Influence of the Nanocrystal Shape Revealed by in-situ Synchrotron SAXS, MRS Fall Meeting & Exhibit 2015, oral presentation, 29.11.-4.12. 2015, Boston, USA
31. L. Ludescher, D. Dirin, G. Fritz-Popovski, M. V. Kovalenko, O. Paris and R.T.Lechner, Chemical and crystalline Structure of spherical and non-spherical CdSe-CdS nanocrystalls, Jahrestagung von ÖPG, SPG, ÖGAA und SGAA in Wien, 01. - 04. September 2015
32. R. Morak, Sorption induced deformation of hierarchical porous silica, SAS2015 16th International Conference on Small-Angle Scattering, 13/09/15 - 18/09/15, Berlin, Germany
33. O. Paris, Hierarchical porous solids and their interaction with molecules and ions, Oskar Paris, International workshop SFB-986 "Hierarchical multiscale materials systems", Hamburg, 4-6.11.2015 **(Invited)**
34. O. Paris, When space becomes tight: Fluid-solid Interactions in Nanoconfinement probed by small-Angle Scattering, O. Paris, SAS 2015, 16th International Conference on Small-Angle Scattering , Berlin, 13.9-18.09.2015 **(Plenary Lecture)**
35. C. Prehal, Tracking the re-arrangement of ions in charged confinement using in-situ X-ray methods, 9th European NESY Winterschool & Symposium on Neutron and Synchrotron Radiation including topical highlight lectures on Neutron and Synchrotron Radiation for Industrial Applications, Altaussee (Austria), March 9-13, 2015 (12 March 2015)
36. C. Prehal, Ion electrosorption studied by in-operando x-ray methods, CDI&E 2015, Saarbrücken Germany 10/2015.
37. C. Prehal, Ion transport in nanoporous carbon supercapacitors tracked by in-situ X-ray methods, ISTP 2015, Leoben Austria 09/2015.
38. C. Prehal, In-situ SAXS and X-ray transmission as complementary tools to study ion electrosorption in charged nanoconfinement, SAS 2015, Berlin Germany 09/2015.
39. C. Prehal, Tracking the global and local ion re-arrangement in carbon nanopores using in-situ X-ray methods, CARBON 2015, Dresden Germany 07/2015.
40. C. Teichert, Growth of small organic molecules on a variety of graphene substrates, Towards Reality in Nanoscale Materials VIII, TRNM, Levi, Finland, 2.-11.2.2015
41. C. Teichert, AVS 62nd International Symposium, IUVSTA High-light Seminar, “Nanometer sized structures are still up-to-date”, San Jose, CA, USA, Oct. 18-23.10.2015. **(Invited)**

42. C. Teichert, AVS 62nd International Symposium, IUVSTA "Sensing Cleanliness of PMMA Transferred CVD Grown Graphene", San Jose, CA, USA, Oct. 18-23.10.2015
43. C. Teichert, 19th Symposium on Condensed Matter Physics - SFKM 2015, "Organic thin film growth on various graphene substrates", Belgrade, Serbia, Sept. 7-11, 2015. **(Invited)**
44. C. Teichert, 8th International Workshop on Nanoscale Pattern Formation at Surfaces, "Ion induced nanopatterning: Understanding and application", Krakow, Poland, July 12 - 16, 2015. **(Invited)**
45. C. Teichert, 2015 International Workshop on Nanomaterials and Nanodevices, "Growth of small organic molecules on a variety of graphene substrates", Beijing, China, June 30 - July 2, 2015. **(Invited)**
46. C. Teichert, International workshop on LEED and related techniques (SPA-LEED 2015), "Facet analysis using Atomic Force Microscopy", Hannover, Germany, May 28-29, 2015.
47. C. Teichert, 8th International NATO Advanced Research Workshop "Functional Nanomaterials and Devices for Electronics, Sensors and Energy Harvesting", "Exploring the growth of organic semiconductors on various graphene substrates for device applications", Lviv, Ukraine, April 13 - 16 2015.
48. C. Teichert, Atomic Force Microscopy Workshop on Advanced Bio- and Materials Characterization and Industrial Applications, "Advanced electrical and nano-mechanical chracterization by AFM", Graz University of Technology + Bruker, Graz, Feb. 18-20 2015. **(Plenary lecture)**

4.2 Invited talks at external institutions: Seminars

1. O. Paris, Hierarchical porous solids and their interaction with fluid matter, Materialwissenschaftliches Kolloquium SFB-986, TU Hamburg Harburg, Germany, 7.11.2014.
2. C. Teichert, "Growth of small organic molecules on graphene", Seminar, Institute of Physics, Academy of Sciences of the Czech Republic, Prag, Czech Republic, 14.11.2014
3. C. Teichert, "Graphene as template for organic thin film growth", Kolloquium aus Physikalischer Chemie, Institut für Oberflächenchemie und Katalyse, Universität Ulm, Germany, 11.11.2014
4. C. Teichert, "Topographic, electric, and photoelectric characterization of inorganic semiconductor nanostructures", Kolloquium, Institut für Halbleitertechnik, Universität Stuttgart, Germany 10.11.2014
5. C. Teichert, "Nanostructure characterization by atomic force microscopy", AFM-Tutorial, Quantum Matter and Materials, Universität zu Köln,Germany, 11.-12.9.2014
6. C. Teichert, "Growth of small organic molecules to sense the cleanliness of various graphene substrates", Seminar, Experimentalphysik, Universität Duisburg Essen, Duisburg, Germany 5.9.2014
7. C. Teichert, "Growth of parahexaphenyl on various graphene substrates", Seminar zur Oberflächenforschung, Institut für Physikalische und Theoretische Chemie, Universität Bonn, Germany 3.9.2014
8. C. Teichert, "Organic thin film growth on graphene and on ion-bombarded rippled substrates", QM²-Kolloquium (Quantum Matter and Materials), Universität zu Köln, Germany 27.8.2014
9. C. Teichert, "Graphene and ion-bombarded, rippled substrates as templates for organic thin film growth", Seminar, Institut für Ionenstrahlphysik und Materialforschung, Helmholtzzentrum Dresden Rossendorf, Germany, 29.7.2014
10. C. Teichert, "Nanomechanical investigation of paper fibers and fiber-fiber joints", Seminar, Max-Planck-Institut für Kolloid- und Grenzflächenforschung, Golm, Germany, 30.6.2014
11. C. Teichert, "Organic thin films on graphene and ion bombarded rutile substrates", Seminar, Oberflächen- und Grenzflächenphysik, Fachbereich Physik, Universität Halle, Halle/Saale, Germany, 16.6.2014
12. C. Teichert, "Parahexaphenyl growth as a sensor to cleanliness of graphene", SFB HIOS-Kolloquium, Department of Physics, Humboldt-University Berlin, Germany, 4.6.2014
13. C. Teichert, "Materialphysik: Von Halbleiternanostrukturen bis hin zu Verpackungspapier", Hautpvortrag, IMST Netzwerk Steiermark, Leoben, Austria 17.1.2014
14. F. Kuchar, Photonic Crystals - From Microwaves to the extreme UV, Seminar, Institute for Microelectronics, TU Wien, Austria, 24.7.2015
15. R. Meisels, Photonik im Bergbau Wie Photonen den Gesteinsabbau leichter machen, Festveranstaltung 30 Jahre Werkstoffe der Elektronik am Institut für Physik der Montanuniversität Leoben, Leoben, Austria, 25.03.2015.

16. O. Paris, When space becomes tight: molecules and ions in nanoconfinement, Department für Materialwissenschaft und Prozesstechnik, Universität für Bodenkultur , Wien, Austria, 17.06.2015.
17. O. Paris, Werkstoffe für Elektronik, Optik und Energie, Festveranstaltung 30 Jahre Werkstoffe der Elektronik am Institut für Physik der Montanuniversität Leoben, Leoben, Austria, 25.03.2015.
18. C. Teichert, "Atomic-force microscopy based exploration of cellulose fibers and wood fiber - nanowire composites, Seminar, Institute of Physics, Academy of Sciences of the Czech Republic, Prag, 22.12.2015
19. C. Teichert, Direkter und indirekter Zugang zu atomaren Oberflächenstrukturen", Seminar, Oberflächen- und Grenzflächenphysik, Fachbereich Physik, Universität Halle, Halle/S. 30.9.2015
20. C. Teichert, "AFM based investigation of graphene substrates", Seminar, Institute for Electron Microscopy and Fine Structure Research (FELMI), Graz University of Technology, Graz, 28.6.2015
21. C. Teichert, Advanced AFM based electrical characterization on the nanometer scale", Seminar, Max Planck Institute of Iron Research Düsseldorf, Germany 27.4.2015
22. C. Teichert, "Growth morphologies of para-hexaphenyl on various graphene and rutile substrates", Seminar, CINAM-CNRS, Marseille, 3.2.2015

4.3 Posters

1. C. Czibula, C. Ganser, A. Miletzky, S. Spirk, R. Schennach, and C. Teichert, AFM studies of adsorbed xylan on amorphous cellulose films using functionalized tips, 64. Jahrestagung der Österreichischen Physikalischen Gesellschaft ÖPG 2014, Pöllau, Austria, 24.-27.9.2014
2. M. Hartmann, Determination of Mechanical Properties of Carbon Nanostructures using Computational Mechanical Tests, 73 IUVSTA Workshop on "Nanostructures on two-dimensional solids, Eisenerz, Austria, 22-26.9.2014
3. S. Klima, M. Mirkowska, M. Kratzer, H. Flachberger, C. Teichert, Studying interaction between mineral particles by atomic force spectroscopy, DPG 2014, Dresden, Germany, 30.3.-4.4.2014
4. Klima, S.; Mirkowska, M.; Kratzer, M.; Flachberger, H.; Teichert, C.:, Contact charging by mineral particles studied by Kelvin Probe Force Microscopy, 64. Jahrestagung der Österreichischen Physikalischen Gesellschaft ÖPG 2014, Pöllau, Austria, 24.-27.9.2014
5. R. Meisels, N. Aoki, R. Akis, D.K. Ferry, R. Brunner Ballistic Transport Characteristic in Single Open Quantum Dots, Arrays and Networks, 18th International Winterschool on New Developments in Solid State Physics, Mauterndorf, Austria, 23.-28.2.2014
6. R. Morak, A simple model to study the influence of topology and distribution of reversible sacrificial bonds on the mechanical behavior of polymers, 64. Jahrestagung der Österreichischen Physikalischen Gesellschaft ÖPG 2014, Pöllau, Austria, 24.-27.9.2014
7. Nevosad, A.; Teichert, C., Inverted bulk-heterojunction solar cell with cross-linked hole-blocking layer, EMRS 2014 Spring Meeting (Symposium C), Lille, France, 26.05.2014
8. J. Oswald, On the imaging of quantum states in the quantum Hall effect regime by scanning gate microscopy, 18th International Winterschool on New Developments in Solid State Physics, Mauterndorf, Austria, 23.-28.2.2014
9. P. Sharifi, Ordered Mesopoirous Thin Films, Elestic Modulus Derminitaion by Humidity Driven Pore Lattice deformation, DFG spring meeting, Dresden, Germany, 30.3.-5.4.2014
10. N. Schrödl, A. Egger, W. Sitte, P. Kreiml, C. Teichert, Investigation of chromium and silicon poisoning of the IT-SOFC cathode material La2NiO4+d., 4. GÖCH-Symposium 2014 "Physikalische Chemie in Österreich". Leoben, Austria, 28.04.2014
11. C. Czibula, C. Ganser, A. Miletzky, S. Spirk, R. Schennach, and C. Teichert, AFM studies of adsorbed xylan on cellulosic materials, DPG 2015, TU Berlin, Germany, 15.-20.3.2015
12. G. Fritz-Popovski, R. Morak, P. Sharifi Rajabi, B. Marmiroli, B. Sartori, H. Amenitsch, O. Paris, Deformation of Microporous Films During Adsorption and Desorption of Water, SAS2015 16th International Conference on Small-Angle Scattering, (16 Sep 2015), Berlin, Germany, 13/09/15 - 18/09/15

13. M. Huszar, T. Kremmer, M. Kratzer, H. Antrekowitsch, and C. Teichert' AFM and KPFM investigation of high strength aluminum brazing sheets, 65. Jahrestagung der Österreichischen Physikalischen Gesellschaft ÖPG 2015, Vienna, Austria,1.-4.9,2015
14. B. Kaufmann, M. Kratzer, T. Lelaidier, O. Siri, A. Matjovic, R. Gajic, C. Becker, C. teichert, Growth morphologies of small polar molecules on SiO_2 and graphene, 65. Jahrestagung der Österreichischen Physikalischen Gesellschaft ÖPG 2015, Vienna, Austria,1.-4.9,2015
15. M. Lasnik**,** S. Röhrig, M. Deluca, M. Kratzer, C. Teichert, Vector piezoresponse force microscopy for analysing the orientation distribution function of ferroelectric domains, 65. Jahrestagung der Österreichischen Physikalischen Gesellschaft ÖPG 2015, Vienna, Austria,1.-4.9,2015
16. R.T. Lechner, L. Ludescher, D. N. Dirin, G. Fritz-Popovski, M. V. Kovalenko, O. Paris, Impact of the Core/Shell Structure of Nanocrystals on the Optical Output Revealed by ASAXS and WAXS, SAS2015 16th International Conference on Small-Angle Scattering, Berlin, Germany,13/09/15 - 18/09/15
17. R. Morak, G. Reichenauer, C. Balzer, N. Hüsing, O. Paris, Comparison of sorption induced deformation of porous materials on different hierarchical levels, NESY 2015, 9th European NESY Winterschool & Symposium on Neutron and Synchrotron Radiation including topical highlight lectures on Neutron and Synchrotron Radiation for Industrial Applications, Altaussee (Austria), March 9-13, 2015
18. R. Morak, F. Putz, M. Elsaesser, G. Fritz-Popovsk, Ch. Balzer, A.M. Waag, N. Hüsing, G. Reichenauer, O. Paris, Structural characterisation and sorption induced deformation of hierarchical silica monoliths with anisotropic porosity, SAS2015 16th International Conference on Small-Angle Scattering, Berlin, Germany,13/09/15 - 18/09/15
19. J. Oswald, 18th International Winterschool on New Developments in Solid State Physics, Mauterndorf, Austria, 12-28.2.2014
20. J. Oswald, Imaging of Condensed Quantum states in the Quantum Halle Effect Regime, 20th International Conference on Magnetism, Barcelona, Spain, 5-10.7.2015
21. C. Prehal, D. Weingarth, H. Amenitsch, V. Presser and O. Paris *Rearrangment of ions in nanoporous carbon supercapacitors studied by in-operando small-angle x-ray scattering,* Pyromanworkshop 2015, Dresden Germany, 10.-11.6.2015

4.4 Awards

- **Lukas Ludescher**: WKO-Forschungsstipendium der WKO Steiermark für die Diplomarbeit: „Über die chemische Struktur von cadmiumselenid (CdSe) / Cadmiumsulfid (CdS) Kern-Schale.Nanokristalle", 6.11.2015
- **Markus Kratzer:** "Best Poster Prize" 8th International Workshop on Nanoscale Pattern Formation at Surfaces, Krakow, Poland, 12.-16.07.2015
- **Christian Prehal:** Student Price oft he Austrian Physical Society (ÖPG-Studierenden-Preis) for his experimental diploma thesis „In-situ SAXS study on the ion dynamics in microporous carbon based supercapacitors" 24.9.2014
- **Christian Prehal:** Rektor-Platzer-Ring, 4.4.2014, Akademischen Feier Montanuniversitaet Leoben
- **Lisa Weniger:** Dr.Hans Riegel-Fachpreis 2015 by the Kaiserschildstiftung 3rd Rank for a VWA based on her experimental work on graphene in the Scanning Probe Microscopy Group of the institute.
- **Christian Koczwara** Förderstipendium für Studierende der Montanuniversität Leoben
- The article "The role of topology and thermal backbone fluctuations on sacrificial bond efficacy in mechanical metalloproteins by **Nabavi et al.** in *New Journal of Physics* 2014" was selected by the editors of *New Journal of Physics* for inclusion in the exclusive "Highlights of 2014" collection
- The article "Tracking the Structural Arrangement of Ions in Carbon Supercapacitor Nanopores Using in Situ Small-Angle X-Ray Scattering" by **C. Prehal,** D. Weingarth, E. Perre, R. T. Lechner, H. Amenitsch, O. Paris, and V. Presser, *Energy & Environmental Science,* **8** (2015), 1725-35 was selected by the editors of *Energy & Environmental Science as "Hot Article" of the month April 2015*

5. Research Projects

5.1 §26 – Projects (FWF-Projects)

Project: **Deformation of hierarchical and anisotropic porous solids by fluid adsorption**
Funded by: FWF (I1605-N20)
Start: 2 June 2014
Duration: 1 June 2017
Project leader: O. Paris
Co-Applicant: N. Hüsing - FB Chemie und Physik der Materialien, Paris-LodronUniversität Salzburg
Internat.Partner G. Reichenauer – Center for Applied Energy Research, Würzburg (DE)
Coworker(s): C. Prehal, L. Ludescher, R. Morak
Funding: € 175.000,-- (only Institute of Physics)

Project: **The role of interfaces for reversible and irreversible deformation of biological materials**
Funded by: FWF (P22983-N20)
Start: 1 Sep 2011
Duration: 30 Jun.2015
Project leader: M. Hartmann
Coworker(s): S.Nabavi
Funding: € 141.000,--

Project: **Growth of polar organic moecules on graphene and saphire**
Funded by: FWF (I 1788-N20 FWF-ANR bilateral project)
Start: 1 Dec. 2014
Duration: 31 March, 2018
Project leader: C. Teichert
Co-Applicant C. Becker, CNRS + University Aix-Marseille, France
Coworker(s): M. Kratzer, A. Matkovic, B. Kaufmann, J. Genser
Funding: € 275.000,--

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: 31 March, 2016
Project leader: T. Antretter (Institut für Mechanik)
Co-Applicant: F. Kuchar, R. Meisels
Funding: € 70.000,-- (inkl. 20% Overhead)

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: 31 Aug 2016
Project leader: M. Deluca (MCL Leoben)
Co-Applicant C.Teichert
Coworker(s): M. Kratzer, M. Lasnik
Funding: € 27.500,--

5.2 §27 – Projects (FFG, EU,…)

Project:	**Hybride Superkondensatoren durch innovative Materialkonzepte** **Programm: Energieforschung (e!MISSION)**
Funded by	Österreichischer Klima- und Energiefonds, FFG Projekt 848808
Start	1.6.2015
Duration	31.5.2018
Project leader	O. Paris
Konsortialpartner	N. Hüsing, - FB Chemie und Physik der Materialien, Paris-LodronUniversität Salzburg
Coworker(s)	C. Prehal, C. Koczwara
Funding:	336.242,-- (only Institute of Physics)

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	01 Sept 2012
Duration	31 May 2014
Project leader	O. Paris
Konsortialpartner	TU Graz – Institut für anorganische Chemie Med Uni Graz - Universitätsklinik für Orthopädie und orthopädische Chirurgie
Coworker(s)	P. Sharifi, C. Ganser, C. Teichert
Funding:	135.854,-- (only Institute of Physics)

Project:	**In-situ SAXS/GISAXS of solid-gas interactions in nanoporous materials and atnanostructured surfaces**
Funded by:	COMET K2 MPPE: Projekt A2.19
Start:	01 Oct 2014
Duration:	July 2016
Project leader:	O. Paris
Project partner(s)	Montanuniversität Leoben, Institut für Physik Materials Center Leoben Forschung GmbH Bruker AXS Analytical X-ray Systems GmbH Montanuniversität Leoben, Lehrstuhl für Materialphysik,
Coworker(s):	R. Morak, G. Popovski C. Prehal
Funding:	Ca 274.000,-- (only Institute of Physics)

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	30. May 2014
Project leader	O. Paris
Coworker(s)	G. Popovski, R. Morak
Funding:	€ 165.000,-- (only Institute of Physics)

5.3 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): F. Schmied, C. Ganser, P. Kreiml, C. Czibula
Funding: € 300.000,--

Project: **CD Labor Faserquellung (Fiber Swelling)**
Funded by: Christian Doppler Gesellschaft
Start: 1. Dec 2015
Duration: Maximum 7 years
Project leader: U. Hirn, TU Graz
Co-Project leader C. Teichert
Coworker(s): C. Ganser, C. Czibula
Funding: € 150.000,--

5.4 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, B. Kaufmann, J. Genser
Funding: € 5.950,--

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: **Nanometer scale electrical investigation of silicon materials for solar energy conversion**
Funded by: ÖAD/ Wissenschaftlich-Technisches Abkommen mit Tschechien, 2014-2015 (Cz Sp 04/2014)
Start: 1 March 2015
Duration: until 29 Feb 2015
Project leader: C. Teichert
Co-Applicant: A. Fejfar, Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic
Coworker(s): M. Kratzer, C. Czibula, J. Genser, K. Gradwohl., L. Kormos
Funding: € 5.388,--

Project: **Two-dimensional materials as templates for the growth of organic semiconductors**
Funded by: ÖAD/ Wissenschaftlich-Technisches Abkommen mit Serbien, 2016-2017 (SRB 09/2016)
Start: Jan 1 2016
Duration: until Dec 31 2017
Project leader: C. Teichert
Co-Applicant: B. Vasic, Institute of Physics, University of Belgrade, Serbien
Coworker(s): M. Kratzer, C. Czibula, J. Genser, K. Gradwohl, B. Kaufmann, A. Matkovic
Funding: € 6.930,--

Project: **Untersuchung der Alterung organischer Dünnschichten auf SiO_2,TiO_2 und Graphen auf der Nanometerskala**
Funded by: ÖAD/ Wissenschaftlich-Technisches Abkommen mit Polen, 2014-2015 (PL 05/2014)
Start: 1 Apr 2014
Duration: until 31 Mar 2016
Project leader: M. Kratzer
Co-Applicant: F. Krok, Institute of Physics, Jagiellonian University, Krakow, Poland
Coworker(s): J. Genser, S. Klima, C. Czibula, C.Teichert
Funding: € 5.231,--

Project: **Nanodraht-Einkristall basierte organisch-inorganische Heterokontakte für Photovoltaik- und Sensorikanwendungen**
Funded by: ÖAD/ Wissenschaftlich-Technisches Abkommen mit der Ukraine, 2015-2016 (UA 07/2015)
Start: 1 Jan 2015
Duration: until 31 Dec 2016
Project leader: M. Kratzer
Co-Applicant: D. Grynko, V. Lashkaryov Insitute of Semiconductor Physics, Kiev, Ukraine
Coworker(s): M. Mirkowska, S. Klima, C. Czibula, C.Teichert
Funding: € 8.000,--

5.5 Funded experiments 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 for synchrotron radiation and neutrons. 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 12 beamtimes. All in all, 60 days of beamtime were granted to the Institute.

2014

Main-proposer	Co Proposer(s)	Proposal Title	Facility	Days
O. Paris	R. Morak H. Amenitsch, B. Marmiroli, B. Sartori (TU Graz)	Humidity driven deformation of mesoporous silica films: the influence of film thickness and film perfection	ELETTRA Triest	5
O. Paris	P. Sharifi J. Meissner, G. Findenegg (TU Berlin) H. Amenitsch (TU Graz)	Bridging aggregation of silica nanoparticles with proteins: kinetics and structure	ELETTRA Triest	5
C. Prehal	C. Prehal, R.T. Lechner V. Presser, D. Weingarth (INM Saarbrücken)	In-situ SAXS study of electrical double layer capacitors: the role of the carbon electrode	ELETTRA Triest	3
O. Paris	C. Prehal, R.T. Lechner V. Presser, D. Weingarth (INM Saarbrücken)	In-situ SAXS study of electrical double layer capacitors: the role of ion size	ELETTRA Triest	6
R.T. Lechner	M. Burian M. Sytnyk, W. Heiss (JKU Linz);	Investigation of the growth of organic hierarchic nanocrystals using a novel synthesis method by in-situ SAXS/WAXS	ELETTRA Triest	6
H.S. Gupta (Queen Mary London)	O. Paris	Microbeam mapping of structure and mechanics of the mineralized cuticle of mantis shrimp telson"	BESSY Berlin	6
				31

2015

R. T. Lechner	O. Paris Maksym Kovalenko (ETH Zürich)	Chemical and crystalline core/shell profile of CdSe/CdS nanocrystals derived by ASAXS and AWAXS	ESRF Grenoble	5
O. Paris	R. Morak N. Hüsing (Univ. Salzburg) G. Reichenauer, C. Balzer (ZAE Würzburg)	Humidity induced deformation of ordered mesoporous silica particles with nanodiffraction and 2D- Ptychography	ESRF Grenoble	4
C. Prehal	O. Paris, C. Koczwara S. Rumswinkel, N. Hüsing (Univ. Salzburg) B. Krüner, V. Presser (INM Saarbrücken)	In-situ SAXS Studies of Electrical Double-Layer Capacitors: the Role of the electrolyte concentration	ELETTRA Triest	5
C. Prehal	O. Paris, C. Koczwara, R.T. Lechner N. Hüsing (Univ. Salzburg), A. Schreiber D. Weingarth, V. Presser (INM Saarbrücken)	In-situ SAXS Studies of Electrical Double-Layer Capacitors: the Ion Structure in Ordered Nanoporous Carbons	ELETTRA Triest	5
G. Reichenauer (ZAE Bayern)	O.Paris C. Balzer (ZAE Bayern)	Sorption induced deformation of a monolithic silica with hierarchical porosity	FRM II München	6
R. T. Lechner	C. Prehal M. Kovalenko (ETH Zürich)	In situ SAXS/WAXS studies of Nanocrystals in Li-ion Battery Anodes	ELETTRA Triest	4
				29

6. Teaching

In the academic year 2014/2015 the number of students registering for Bachelor studies at the Montanuniversität Leoben raised to an all-time maximum of more than 700, which means an increase of more than 30% as compared to the previous year. This was putting a never seen pressure to the whole Institute of Physics in terms of lecturing, examination and administration in basic phyiscs. We are also strongly involved in the Master Curriculum Materials Science, in particular with the “Wahlfachgruppe: Materials for Electronics and Physics of Functional Materials”. Two new lectures were established within the reporting period, i.e., “Solar Cells” by R. Brunner and “Introduction into Synchrotron Radiation” by O. Paris. The latter was introduced to support the very successful on-site practical training at the synchrotron radiation source ELETTRA, which has found its way into the Materials Science Master curriculum into two “Wahlfachgruppen”.

6.1 Courses held in the years 2014 and 2015

Winter Term 2013/2014

Number	**Title**	**Hours per week / Type**		**Lecturer**
460.129	Anleitung zu wissenschaftlicher Arbeit auf dem Gebiet der Physik von Halbleitern und Nanosystemen	8	PV	Meisels R, 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
460.066	Industrielle Herstellungstechniken der Mikroelektronik	2	VO	Ganitzer P
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 *(17 groups)*	2	UE	Hartmann M, Kratzer M, Lechner R, Meisels R, Morak R, Oswald J, Popovski G, Teichert C, Wurster S
460.114	Quantenmechanik *(1 group)*	2,5	IV	Oswald J
460.001	Rechenübungen zu Physik IA und IB *(21 groups)*	2	UE	Angerer P, Battisti M, Bodor C, Ganser C, Hartmann M, Hofstätter M, Klünsner T, Kratzer M, Lechner R.T, Meisels R, Morak R, Moser A, Popovski G, Teichert C, Waldner P
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
460.200	Seminar Bachelorarbeit	4	SE	Meisels R, Oswald J, Paris O, Teichert C
460.070	Solarzellen	2	VO	Brunner R

Summer Term 2014

Number	Title	Hours per week / Type		Lecturer
460.132	Anleitung zu wissenschaftlicher Arbeit auf dem Gebiet der Physik von Halbleitern und Nanosystemen	4	PV	Paris O, Teichert C
460.108	Anwendung von Computersimulationen in der Metall- und Biophysik	2	VO	Hartmann M
460.461	Einführung in die Synchrotronstrahlung	1	VO	Paris O
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 *(8 groups)*	2	UE	Hartmann M, Kratzer M, Lechner R.T, Meisels R, Morak R, Oswald J
460.113	Physik von Fullerenen, Graphen und Carbon Nanotubes	2	VO	Teichert C
460.069	Physikalische Messtechnik *(3 groups)*	2	IV	Meisels R, Oswald J
460.103	Rastersondentechniken zur Charakterisierung von Festkörperoberflächen	2	VO	Teichert C
460.009	Rechenübungen zu Physik II *(18 groups)*	1	UE	Angerer P, Hartmann M, Hofstätter M, Klünsner T, Kratzer M, Lechner R.T, Meisels R, Morak R, Moser A, Popovski G, Waldner P
460.048	Rechenübungen zu Physik III	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
460.462	Synchrotronstrahlung in der Materialforschung	2	UE	Lechner R, Paris O
420.102	Einführung in die Werkstoffwissenschaft	0,1875	SE	Paris O., Teichert C.
430.001	Werkstoffmodellierung auf atomarer Ebene	0,67	VO	Hartmann M.
430.101	Übungen zu Werkstoffmodellierung auf atomarer Ebene	0,66	UE	Hartmann M.

Winter Term 2014/2015

Number	Title	Hours per week / Type		Lecturer
460.129	Anleitung zu wissenschaftlicher Arbeit auf dem Gebiet der Physik von Halbleitern und Nanosystemen	8	PV	Meisels R, 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
460.066	Industrielle Herstellungstechniken der Mikroelektronik	2	VO	Ganitzer P

460.003	Konversatorium zu Physik I	1	KV	Paris O
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 *(16 groups)*	2	UE	Ganser C, Hartmann M, Kratzer M, Lechner R.T, Meisels R, Oswald J, Teichert C
460.114	Quantenmechanik *(2 groups)*	2,5	IV	Oswald J
460.001	Rechenübungen zu Physik IA und IB *(25 groups)*	2	UE	Angerer P, Brunner R, Ganser C, Grundner K, Hartmann M, Hofstätter M, Kratzer M, Lechner R.T, Meisels R, Morak R, Popovski G, Prehal C, Putz B, Teichert C, Waldner P, Wießner M
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
460.070	Solarzellen	2	VO	Brunner R
460.076	Übungen zu Charakterisierung von Werkstoffen der Elektronik	2	UE	Lechner R, Meisels R, Oswald J, Teichert C

Summer Term 2015

Number	**Title**	**Hours per week / Type**		**Lecturer**
460.132	Anleitung zu wissenschaftlicher Arbeit auf dem Gebiet der Physik von Halbleitern und Nanosystemen	6	PV	Meisels R, Paris O, Teichert C
460.108	Anwendung von Computersimulationen in der Metall- und Biophysik	2	VO	Hartmann M
460.461	Einführung in die Synchrotronstrahlung	1	VO	Paris O
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.T
460.010	Physik II	2	VO	Paris O
460.016	Physik III	2	VO	Teichert C
460.054	Physik Praktikum II *(7 groups)*	2	UE	Kratzer M, Meisels R, Morak R, Oswald J
460.113	Physik von Fullerenen, Graphen und Carbon Nanotubes	2	VO	Teichert C
460.069	Physikalische Messtechnik *(5 groups)*	2	IV	Meisels R, Oswald J
460.103	Rastersondentechniken zur Charakterisierung von Festkörperoberflächen	2	VO	Teichert C
460.009	Rechenübungen zu Physik II *(23 groups)*	1	UE	Angerer P, Brunner R, Eck S, Grundner K, Hofstätter M, Kaufmann B, Kratzer M, Lechner R.T, Meisels R, Morak R, Popovski G, Prehal C, Putz B, Waldner P, Wießner M

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
460.100	Strukturforschung mit Röntgen- und Neutronenstreuung an Europäischen Großforschungsanlagen	2	VO	Keckes J, Paris O
460.462	Synchrotronstrahlung in der Materialforschung	2	UE	Lechner R.T, Paris O
420.102	Einführung in die Werkstoffwissenschaft	0,1875	SE	Paris O., Teichert C.
430.001	Werkstoffmodellierung auf atomarer Ebene	0,67	VO	Hartmann M.
430.101	Übungen zu Werkstoffmodellierung auf atomarer Ebene	0,66	UE	Hartmann M.

Winter Terms 2015/2016

Number	**Title**	**Hours per week / Type**		**Lecturer**
460.129	Anleitung zu wissenschaftlicher Arbeit auf dem Gebiet der Physik von Halbleitern und Nanosystemen	8	PV	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
460.066	Industrielle Herstellungstechniken der Mikroelektronik	2	VO	Ganitzer P
460.003	Konversatorium zu Physik I	1	KV	Paris O
460.072	Physik der Mikro- und Nanoelektronik-Bauelemente	2	VO	Meisels R
460.007	Physik IA	1,75	VO	Paris O
460.008	Physik IB	1,75	VO	Paris O
460.030	Physik Praktikum I *(18 groups)*	2	UE	Ganser C, Kratzer M, Lechner R.T, Meisels R, Morak R, Oswald J, Popovski G
460.000	Physik 0	0,5	IV	Paris O
460.114	Quantenmechanik *(2 groups)*	2,5	IV	Oswald J
460.001	Rechenübungen zu Physik IA und IB *(24 groups)*	2	UE	Angerer P, Brunner R, Eck S, Ganser C, Hofstätter M, Kaufmann B, Koczwara C, Kratzer M, Lechner R.T, Morak R, Prehal C, Putz B, Teichert C, Waldner P, Wießner M
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
460.200	Seminar Bachelorarbeit	4	SE	Paris O, Teichert C
460.070	Solarzellen	2	VO	Brunner R

6.2 Lectors: External help with teaching

Since a long time it is a tradition that temporary external lecturers are associated with the Institute of Physics. They particularly help us to cover the exercises and the practical training in Physics for the ever increasing number of freshmen students. The table below demonstrates that in the meanwhile the numbers include up to 25 exercise groups and up to 18 groups in the practical training which have to run in parallel each semester. It is clear that this large number of groups cannot be run by the faculty staff, even though the two Senior Lecturers do cover an enormous part of the paractical training.

We are therefore very gratefully for the continuous help from third party funded research associates coming either from our own Institute, from other Chairs of the Montanuniversität, or from external institutions, e.g., the Materials Center Leoben (MCL) or the Erich Schmid Institute of the Austrian Academy of Sciences (ESI-ÖAW)

- Dr. C. Ganser, MSc. B. Kaufmann, MSc. S. Nabavi, Dipl.Ing., C. Prehal, Dr. G. Popovski, Institut für Physik
- Dr. M. Hofstätter, Institut für Struktur- und Funktionskeramik
- Dr. P. Angerer, Dr. S. Eck, Doz. Dr. R. Brunner, Dr. T. Klünsner, Dr. M. Wießner, Materials Center Leoben
- Dipl.Ing. K. Grundner, Dipl.Ing. B. Putz , Dipl. Ing. S. Wurster, Lehrstuhl für Materialphysik & ESI-ÖAW
- Dipl.Ing. C. Bodor, Lehrstuhl für Spritzgießen von Kunststoffen
- Dr. M. Battisti, Lehrstuhl für Kunststoffverarbeitung
- Dipl.Ing. A. Moser, Lehrstuhl für Werkstoffkunde und Prüfung der Kunststoffe
- Doz. Dr. P. Waldner, Lehrstuhl für Physikalische Chemie

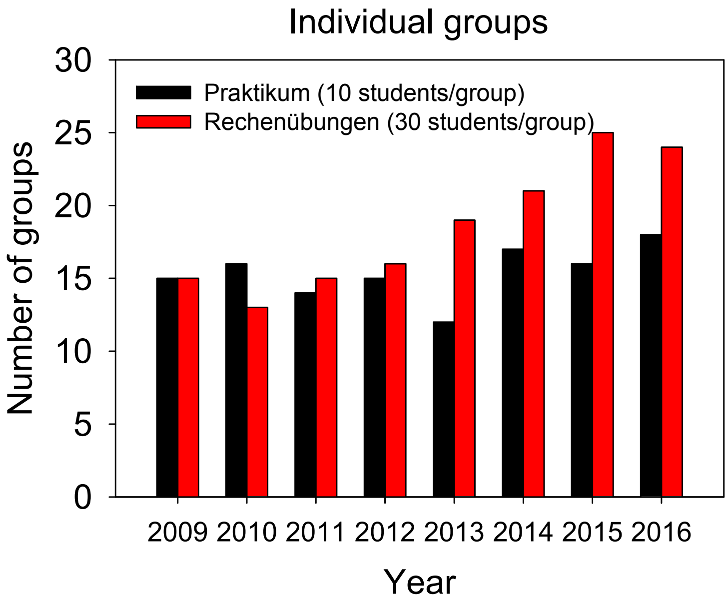
In addition, we are very grateful to

- Univ.Prof. Dr. E. Kasper, Institut für Halbleitertechnik, Universität Stuttgart, Germany
- Dr. P. Gantitzer, Infineon Technologies Austria AG, Villach
- Doz. Dr. R. Brunner, Materials Center Leoben

who support the Institute by delivering important lectures in the “Wahlfachgruppe: Werkstoff der Elektronik und Physik funktionaler Materialien”.

Also the help of the SAXS Beamline group at the ELETTRA synchrotron radiation source in Trieste with the on-site practical training within the course “Synchrotron Radiation in Materials Science” is gratefully acknowledged

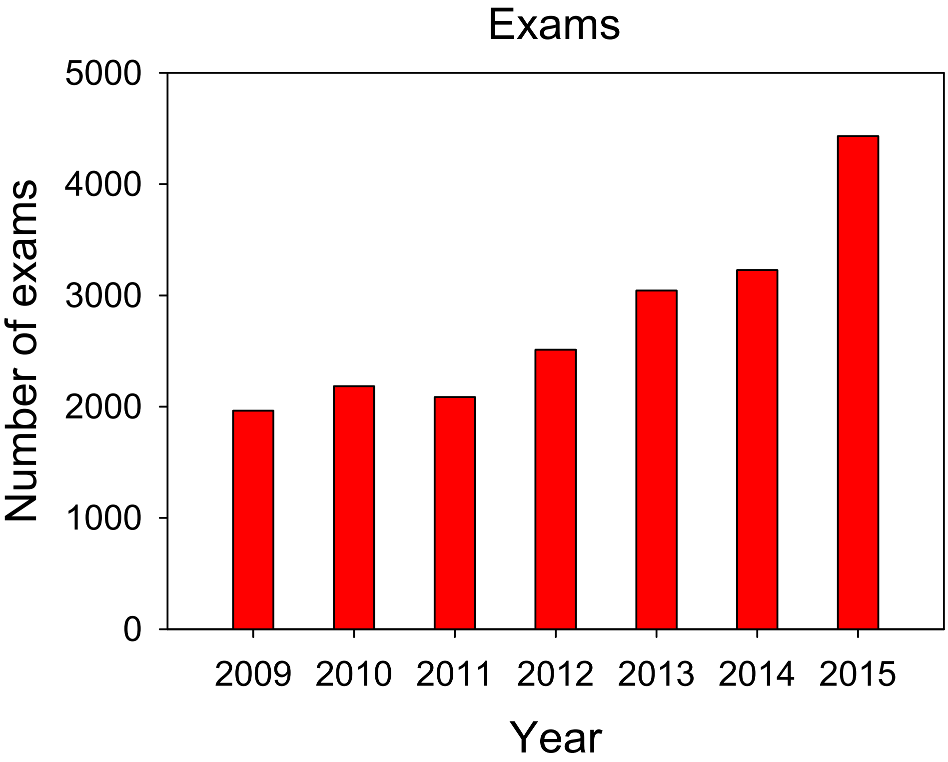
- Dr. H. Amenitsch, Dr. B. Marmiroli, Dr. B. Sartori, Institute of inorganic Chemistry, TU Graz.



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 increased only slightly within the last years, the number of classes for the exercises has increased by more than 50%.

6.3 Exams

LV.Nr.	Titel	2012	2013	2014	2015
460.000	Physik 0				482
460.001	Rechenübungen zu Physik IA & IB	485	627	573	709
460.002	Physik I	83	1	0	0
460.003	Konversatorium zu Physik I	56	0		65
460.004	Repetitorium Physik I	23	14	14	20
460.005 460.007	Physik IA	463	703	782	860
460.006	Physik IB	239	394	431	637
460.009	Rechenübungen zu Physik II	402	494	498	580
460.010	Physik II	238	331	359	522
460.016	Physik III	63	39	52	53
460.030	Physik Praktikum I	150	123	156	156
460.048	Rechenübungen zu Physik III	52	31	44	47
460.054	Physik Praktikum II	61	48	77	65
460.060	Bauprinzipien biologischer Materialien	32	36	25	26
460.066	Industrielle Herstellungstechniken der Mikroelektronik	3	0	1	4
460.067	Mechanisch-Physikalische Messtechnik	38	49	57	19
460.068	Übungen zu Mechanisch-Physikalische Messtechnik	33	38	1	0
460.069	Physikalische Messtechnik			23	43
460.070	Solarzellen			10	9
460.072	Physik der Mikro- und Nanoelektronik-Bauelemente	1	1	1	
460.076	Übungen zu Charakterisierung von Werkstoffen der Elektronik	0	1	0	0
460.077	Physikalische und Technische Grundlagen von Sensoren	1	0	0	0
460.094	Halbleiterwerkstoffe	34	26	51	33
460.100	Strukturforschung mit Röntgen- und Neutronenstreuung an Europäischen Großforschungsanlagen	0	6	0	5
460.102	Elektronische und mechanische Eigenschaften von Heterostruktur-Bauelementen	0	0	3	1
460.103	Rastersondentechniken zur Charakterisierung von Festkörperoberflächen	12	6	7	10
460.104	Herstellung einkristalliner Schichten - Epitaxie	0	2	4	5
460.105	Magnetische Eigenschaften von Nanowerkstoffen	1	0	2	0
460.108	Anwendung von Computersimulationen in der Metall- und Biophysik	3	0	3	2
460.110	Grundprinzipien der Quantenphysik	1	0	0	1
460.111	Einführung in die Oberflächen- und Dünnschichtprozesse	7	3	4	7
460.113	Physik von Fullerenen, Graphen und Carbon Nanotubes	2	6	3	2
460.114	Quantenmechanik	0	49	34	46
430.001	Werkstoffmodellierung auf atomarer Ebene	2	3		
460.460 460.462	Exkursion: Synchrotronstrahlung in der Materialforschung / Synchrotronstrahlung in der Materialforschung	21	10	8	9
460.461	Einführung in die Synchrotronstrahlung				5
	Bachelorprüfungen				3
	Diplomprüfungen	2	1	2	1
	Total number of exams	**2.508**	**3.042**	**3.225**	**4.427**



The diagram shows the development of the annual number of exams taken by the Institute of Physics. As compared to 2009-2011 this number has essentially doubled. Asuming 15 minutes as an absolute minimum time for each single exam, 4.427 exams amount to more than 1.100 hours of examination, which comes to 138 full working days or about 4.5 months/year of sole examination time.

7. Bachelor-, Diploma- and Doctoral Theses

7.1 Bachelor Theses

Konstantiniuk, Fabian Supervisor: C. Teichert Finished: Nov. 2015	Roughness analysis of silane coating metal surfaces by atomic force microscopy
Kappacher, Johann Supervisor: R. Brunner, O. Paris Finished: Nov. 2015	Evaluation of non-destructive scanning acoustic microscopy for the charakterisation of microstructural damage in high alloy bearing steel
Pfleger, Bernd Supervisor: C. Teichert Finished: Nov. 2015	Kelvin Probe Force Microscopy of Yttrium Barium Copper Oxide

7.2 Diploma Theses

Michael HUSZAR Supervisor: C. Teichert Since: June 2015	AFM and KPFM investigation of high-strength Aluminium brazing sheets
Jakob Alexander GENSER Supervisor: C. Teichert Since: Oct 2015	Growth of para-hexaphenyl on exfolieted hexagonal boron nitride flakes
Patrice KREIML Supervisor: C. Teichert Finished: March: 2016	Investigation of water absorption of cellulose fibers by gravimetric analysis and atomic force microscopy
Michael LASNIK Supervisor: C. Teichert, M. Kratzer, M. Deluca Finished: Feb 2016	Determination of the Orientation Distribution Function of PZT Ceramics by Piezoresponse Force Microscopy
Lukas LUDESCHER Supervisor: R.T. Lechner, O. Paris Finished: March: 2016	On the chemical and crystalline structure of CdSe/CdS core-shell nanocrystals
Caterina CZIBULA Supervisor: C. Teichert Finished: June 2016	Exploring chemical contrast on cellulosic materials with atomic force microscopy
Stefan KLIMA Supervisor: C. Teichert Finished: June 2015	Charging of calcite(100) surface by contact with mineral particles studied by Kelvin Probe 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

7.3 Doctoral Theses

Christian KOCZWARA Supervisor: O. Paris Since: Sept 2015	Hybrid supercapacitors
Christian PREHAL Supervisor: O Paris Since: April 2014	Ionen in begrenzter Geometrie sowie elektrosorptionsinduzierte Phänomene
Benjamin KAUFMANN Supervisor: C. Teichert Since: Feb 2015	Growth of Small Polar Molecules on Graphene and Sapphire
Roland J. MORAK Supervisor: O. Paris Since: Oct 2013	Wechsewirkung von Flüssigkeiten und Gasen mit Festkörpern in hochporösen Systemen
Seyedsoran NABAVI Supervisors: O. Paris & M. Hartmann Finished: March 2015	Understanding Interfaces in Biological Tissue
Christian GANSER Supervisor: C. Teichert Finished:March 2015	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
Michael TOIFL Supervisor: T.Antretter R. Meisels Since: July 2013	Numerical study of microwave induced stress and damage formation in heterogeneous rocks

7.4 Habilitation Theses

Roland BRUNNER Finished: May 2014	Beyond CMOS: Towards Semiconductor Based Quantum Information Processing

8. Incomings: Invited Guests (Seminar)

2014

Thu, 18. December 2014
(together with the
Department Allgemeine
Analytische und
Physikalische Chemie)

Kolloquium zu den Nobelpreisen 2014

Prof. Dr. Henning Riechert
(Direktor des Paul Drude Instituts für Festkörperelektronik, Berlin)
„Galliumnitrid LED - die Beleuchtung des 21. Jahrhunderts“
Der Nobelpreis für Physik 2014 geht an die drei japanischen Wissenschaftler **Isamu Akasaki, Hiroshi Amano und Shuji** Nakamura (jetzt USA) für die „Erfindung effizienter, blaues Licht ausstrahlender Dioden, die helle und energiesparende weiße Lichtquellen ermöglicht haben“.

Univ.-Prof. Dr. Thomas Klar
Institut für Angewandte Physik, Johannes Kepler Universität Linz
„Mikroskopieren, besser als Abbe erlaubt "
Der **Nobelpreis für Chemie 2014** geht an **Eric Betzig (USA), Stefan W. Hell (Deutschland, geb. in Rumänien)** und **William E. Moerner (USA)** für die „Entwicklung von superauflösender Fluoreszenzmikroskopie“, mit der die bisherige Abbe´sche Auflösungsgrenze der optischer Mikroskopie radikal unterlaufen werden kann.“

Thu, 16. December 2014

Dr. Maksym Yarema
(Laboratory for Nanoelectronics, ETH Zurich, Zurich, Switzerland)
“**Superposition of composition and size effects in colloidal I-III-VI quantum dots”**

Tue, 9. December 2014

Soran Nabavi
(Institut für Physik, Montanuniversität Leoben)
"The role of reversible cross-links on the mechanical properties of polymeric systems- A Monte Carlo study”

Tue, 2. December 2014

Dr. Christian Ganser
(Institut für Physik, Montanuniversität Leoben)
“Humidity influence on the mechanical properties of cellulosic materials determined by AFM based nanoindentation”

Thu, 27. November 2014

Dr. Richard Weinkamer
(Max-Planck-Institut für Kolloid- und Grenzflächenforschung Wissenschaftspark Golm, Abteilung Biomaterialien, Potsdam, Germany)
"Structural adaptation of bone"

Tue, 25. November 2014

Dr. Harald Plank
(Institute for Electron Microscopy and Nanoanalysis, Graz University of Technology, Graz, Centre for Electron Microscopy, Graz, Austria)
"Advanced FIB / FEB Dual Beam Prototyping & Real Time AFM in Biology"

Tue, 11. November 2014

em.O.Univ.Prof. Dr. Friedemar Kuchar
(Institut für Physik, Montanuniversität Leoben)
"Zukünftige Tendenzen in der Halbleitertechnologie und der Computer gestützten Materialmodellierung"

Tue, 17. June 2014

Prof. Dr. Rudolf A Roemer
(Centre for Scientific Computing or Department of Physics University of Warwick, Coventry CV4 7AL UK)
"From disorder, graphene and interacting quantum many-body systems to the rigidity and flexibility of PDI and HIV protease"

Thu, 5. June 2014

Dr. Igor Beinik
(Interdisciplinary Nanoscience Center - INANO-Fysik, iNANO-huset, Aarhus , Danmark)

"The microscopic view on the thermally induced interaction of Cu with ZnO"

Mon, 2. June 2014
Prof. Dr. Leszek Markowski
(Institute of Experimental Physics, University of Wroc?aw, Wroc?aw, Poland)
"On the Reverse Problem and Some Quantum Effects in Ion Desorption from Ionic Crystals"

Tue, 27. May 2014
Univ.Prof. Dr. Wolfgang Lang
(Fakultät für Physik der Universität Wien, Elektronische Materialeigenschaften)
„Swift and lazy vortices in cuprate high-T_c superconductors"

Tue, 20. May 2014
Prof. Dr. Tomáš Šikola
(Fakulty of Mechanical Engineering, Institute of Physical Engineering, Dept. of Solid State Physics and Surfaces, CEITEC, Brno University of Technology, Brno, Czech Republic)

Wed, 23. April.2014
Dr. Michaela Eder
(Max Planck Institut für Kolloid- und Grenzflächenforschung, Potsdam)
"Fire, rain and dryness trigger seed release"

Tue, 25. March.2014
Dr. Oleg Dimitriev
(V.Lashkaryov Institute of Semiconductor Physics, Nauki , Kiev, Ukraine)
Application of CdS nanostructured layers in hybrid solar cells: Effect of the layer morphology and dye sensitizer on photovoltaic performance

Tue, 18. March 2014
Univ.Prof. Dr. Armando Rastelli
(Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz)
"Strain-tunable quantum optoelectronic devices"

Fri, 24. January 2014
Prof. Dr. Franciszek Krok
(Institute of Physics, Jagiellonian University, Krakow, Poland)
„Atomic-scale friction on stepped surfaces of single crystal semiconductors"

Tue, 14. January 2014
Prof. Dr. Nicola Hüsing
(Materials Science and Physics, Paris-Lodron University Salzburg)
"Highly porous functional materials - sometimes less is more -"

2015

Thu, 17. December 2015 (together with the Department Allgemeine Analytische und Physikalische Chemie)

Kolloquium zu den Nobelpreisen 2015

Prof. Dr. Thomas Schwetz-Mangold
Institut für Nuklearphysik, Karlsruhe Institut für Technologie (KIT)
Neutrinos: Geisterteilchen in Kosmologie und Elementarteilchenphysik
Der Nobelpreis für Physik 2015 geht an **Takaaki Kajita** (University of Tokyo, Japan) und **Arthur B. McDonald** (Queen's University, Kingston, Kanada) **„für die Entdeckung der Neutrinooszillation, die zeigt, dass Neutrinos Masse besitzen"**.

Univ.-Prof. Dr. Kai-Uwe Fröhlich
Institut für Molekulare Biowissenschaften, Karl-Franzens Universität Graz
Wer kontrolliert die Kontrolleure?
- Unsere Chemie-Nobelpreisträger 2015
Der Nobelpreis für Chemie 2015 geht an **Tomas Lindahl** (Francis Crick Institute, London, Großbritannien), **Paul Modrich** (Howard Hughes Medical Institute, Chevy Chase, USA) und **Aziz Sancar** (University of North Carolina, USA) für **„die Entschlüsselung des Prozesses wie Zellen beschädigte DNA reparieren und dabei genetische Informationen sichern".**

Tue, 15. December 2015	**Dr. Daniel Van Opdenbosch** *(TU München, Fachgebiet Biogene Polymere, Straubing, Germany)* **Phototactic structuring of polysaccharide biotemplates by micro-algae“**
Thu, 10. December 2015	**Prof. Dr. Thomas Ihn** (Solid State Physics Laboratory, ETH Zürich, Schweiz) **„Investigating quantum circuits using scanning-gate techniques“**
Tue, 1. December 2015	**Priv.-Doz. Elisabeth Soergel**, *(Institut für Physik, Rheinische Friedrich-Wilhelms-Universität Bonn)* **"Piezoresponse force microscopy: from imaging ferroelectric domains towards a quantitative characterization of ferroelectrics"**
Tue, 24. November 2015	**Dr. Bernhard Bayer** *(Faculty of Physics, University of Vienna, Austria)* **”Scalable growth and integration of low-dimensional nanomaterials”**
Tue, 10. November 2015	**Univ.Prof. Dr. Julian Stangl** *(Institut für Halbleiter- und Festkörperphysik, Johannes Kepler Universität Linz)* ***"X-ray diffraction as local strain probe and for crystallography of semiconductor nanostructures"***
Fri, 16. October 2015	**Dr. Wolfgang Wagermaier** (Max Planck Institute of Colloids and Interfaces, Potsdam, Germany) **”Characterizing structure and properties of bone and bioinspired materials by a multi-method approach”**
Tue, 6. October 2015	**Dr. Thomas Müller** *(Institut für Photonik, TU Wien)* **"Optoelectronics in two-dimensional atomic crystals”**
Tue, 9. June 2015	**Ass.Prof. Dr. Stefan Spirk** *(Institut für Chemische Technologie von Materialien, TU Graz)* **Cellulosic Substrates as Supports for Advanced Materials**
Tue, 24. March 2015	**Dr. Davide Ruffoni** (University of Liége, Dept.of Aerospace and Mechanical Engineering, Liége, Belgium) **Bone remodeling and mineralization investigated by four-dimension micro-computed tomography**
Tue, 3. March 2015	**Prof. Dr. Maksym V. Kovalenko** *(ETH Zürich, Department of Chemistry and Applied Biosciences, Zurich, and Empa-Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland)*Novel Strategies for Combining **"Molecules, Clusters, and Nanocrystals into Functional Inorganic Solids"**
Tue, 27. January 2015	**Prof. Dr. Patrick Huber** (Hamburg University of TechnologyInstitute of Materials Physics and Technology, Hamburg, Germany) **Soft Matter in Hard Confinement: How molecular condensates arrange, diffuse and flow in nanoporous media**

9. Outgoings: Foreign Research Visits of Institute Members

M. Burian	07.04.2014 – 13.04.2014	SAXS Beamline, Synchrotron ELETTRA Trieste (Italien)
	25.05.2014 – 28.05.2014	SAXS Beamline, Synchrotron ELETTRA Trieste (Italien)
K.P. Gradwohl	06.09.2015 - 13.09.2015	Institut für Physik der Tcschechischen Akadmie der Wissenschaften, Prag (Tschechien), Forschungsaufenthalt im Rahmen des ÖAD Projektes CZSP/2014
C. Koczwara	18.10.2015 - 22.10.2015	Elekjtrochemische Messungen am INM – Leibnitz-Institut für Neue Materialien, Saarbrücken (Germany)
	12.11.2015- 18.11.2015	SAXS Beamline, Synchrotron ELETTRA Trieste (Italien)
M. Kratzer	30.06.2014- 06.07.2014	CINAM-CNRS Marseille (France), Forschungsaufenthalt im Rahmen des ÖAD Projektes FR17/2013
	15.12.2014- 19.12.2014	Institute of Physics, Jagellonian University Krakow (Poland)
	13.12.2015- 18.12.2015	Institute of Physics, Jagellonian University Krakow (Poland)
R. T. Lechner	07.04.2014 – 13.04.2014	Synchrotron ELETTRA, Sincrotrone Trieste (Italy)
	25.05.2014 – 28.05.2014	SAXS Beamline, Synchrotron ELETTRA Trieste (Italien)
	26.02.2015 - 02.03.2015	European Synchrotron Radiation Facility - ESRF (France)
	01.11.2015 – 06.11.2015	Synchrotron ELETTRA, Sincrotrone Trieste (Italy)
L. Ludescher	05.20.2015 - 11.10.2015	MLZ Garching, FRM 2, Messzeit DIANA (Germany)
	10.11.2015 – 18.11.2015	Messzeit ESRF, Grenoble (France)
R. Morak	10.09.2014 – 16.09.2014	SAXS Beamline, Synchrotron ELETTRA Trieste (Italien)
	05.10.2015 - 12.10.2015	Research Reactor FRM II, Garching,Munich (Germany)
O. Paris	08.10.2015 - 12.10.2015	Research Reactor FRM II, Garching,Munich (Germany)
C. Prehal	08.05.2014 – 14.05.2014	SAXS Beamline, Synchrotron ELETTRA Trieste (Italien)
	25.05.2014 – 28.05.2014	SAXS Beamline, Synchrotron ELETTRA Trieste (Italien)

	12.11.2015- 18.11.2015	SAXS Beamline, Synchrotron ELETTRA Trieste (Italien)
C. Teichert	04.04.2014 - 09.04.2014	Institute of Physics, Jagiellonian University, Krakow (Polen) Forschungsaufenthalt im Rahmen des ÖAD Projektes PL19/2012
	21.06.2014 – 18.07.2014	Universitaet Köln, (Germany)
	19.07.2014 – 17.08.2014	Martin Luther Universitaet Halle-Wittenberg (Germany)
	18.08.2014 – 20.09.2014	Universitaet Köln, (Germany)
	02.02.2015 - 04.02.2015	CINAM-CNRS, Marseille (France), Forschungsaufenthalt im Rahmen des ÖAD Projektes FR17/2013
	13.04.2015 - 17.04.2015	Taras Shevchenko National University of Kyiv, Physics Dempartment, Lviv (Ukraine) Forschungsaufenthalt im Rahmen des ÖAD Projektes UA11/2013
	12.07.2015 – 17.07.2015	Forschungsaufenthalt im Rahmen des ÖAD Projektes PL05/2014

10. Conference Organisation

Organisation of Conferences, Workshops or Schools

Oskar Paris

- CISM course "Structure and Multiscale Mechanics of Carbon Nanomateirals, July 21-25, 2014 Udine, Italy
- Festveranstaltung: 30 Jahre Werkstoffe der Elektronik am Institut für Physik der Montanuniversität Leoben, 25.03.2015
- Tag der Lehre 2015, Montanuniversität Leoben, 04.12.2015.

Rainer T. Lechner & Oskar Paris

9th European NESY Winter-School & Symposium on Neutrons and Synchrotron Radiation including topical highlight lectures on Neutron and Synchrotron Radiation for Industrial Applications, Altaussee (Austria), March 9-13, 2015, Austria

Friedemar Kuchar, G. Bauer, W. Jantsch

18th International Winterschool on New Developments in Solid State Physics, Feb 23 – 28, 2014, Castle of Mauterndorf, A-5570 Mauterndorf, Province of Salzburg, Austria

Christian Teichert

73rd IUVSTA Workshop “Nanostructures on two-dimensional solids”, 22. – 26.9. 2014, Eisenerz, Austria

Organisation of Symposia or Sessions at Conferences

Oskar Paris

- Oskar Paris & Martin Müller (Helmholtzzentrum Geesthacht) : DPG Frühjahrstagung, Fachverband Metall- und Materialphysik, Organisation eines fachinternen Symposiums " X-ray and Neutron Scattering in Materials Science„ 1.-4. April 2014, Dresden

- Oskar Paris & Richard Weinkamer (MPI Kolloid- und Grenzflächenforschung Potsdam), & Regine Willumeit (Helmholtzzentrum Geesthacht): DPG Frühjahrstagung, Fachverband Metall- und Materialphysik, Organisation eines fachinternen Symposiums "Biomaterials and Biological Materials, 30.3-4.4.2015, Berlin.
- Oskar Paris: NESY Session, bei der Jahrestagung der Österreichischen Physikalischen Gesellschaft, Sept 24-26, 2014, Pöllau, Austria

Mitgliedschaften in Programmkommittees & Advisory Boards von Tagungen

Oskar Paris

- Member International Advisory Board: Bioinspired Materials Conference, 22.-25.2.2016, Potsdam
- Member Scientific Program Committee: International conference on Small-angle scattering (SAS 2015, 13.-18.9.2015, Berlin
- Member International Advisory Board: Bioinspired Materials Conference, 18.-21.3.2014, Potsdam
- Organizing Committee: Research at European Neutron and Synchrotron Facilities by Austrian Researchers, 11.-12.11.2013, TU Wien.

Christian Teichert

- Member International Program Committee 75th IUVSTA Workshop “Structures of ultrathin films of oxides on metal surfaces”, Avila, Spain, July 6 - 12 2015.
- Member International Steering Committee, Intl. Conference on Nanoscience + Technology (ICN+T 2014), Vail, CO, USA, July 23-27, 2014.
- Member International Program Committee, 8th International Workshop on Nanoscale Pattern Formation at Surfaces, Krakow, Poland, July 12 – 16, 2015.
- Member International Program Committee, 19th International Winterschool on New Developments in Solid State Physics, Mauterndorf, Feb. 21 - 26, 2016.
- Vice-Chair Organizing Committee and Member Program Committee, 14th IUVSTA School on Nano-Optics, Braga, Portugal, Apr. 11- 15, 2016.
- Member International Steering Committee, Intl. Conference on Nanoscience + Technology (ICN+T 2016), Busan, South Korea, Aug. 21 - 26, 2016.
- Co-Chair International Scientific Committee “Nanometer Structures” IVC-20, Busan, South Korea, Aug. 21 - 26, 2016

Markus Kratzer

Member of the Organizing Committee des 73 IUVSTA Workshop on “Nanostructures on two-dimensional solids”, Eisenerz, Österreich, Sept. 22-26, 2014

11. University Administration

Oskar Paris (MUL)

- Institutsvorstand (Chair): since 2009
- Vizestudiendekan: since 2011
- Curriculumskommission Werkstoffwissenschaften (Member)
- Curriculumskommission Kunststofftechnik (substitute member)
- Berufungskommission Materialphysik 2013-2014 (Member)
- Berufungskommission Reservoir Engineering 2015 (Member)
- Habilitationskommission Griesser 2014 (Member)
- Habilitationskommission Brunner 2014 (Member and Reviewer)
- Habilitationskommission Gruber 2015 (Member and Reviewer)
- Habilitationskommision Holec 2015/16 (Member)
- Habilitationskommision Deluca 2015/16 (Member)

Ronald Meisels
- Curriculumskommission „Doktoratsstudium“

Rainer T. Lechner
- Sicherheitsvertrauensperson (SVP): since 2012

Josef Oswald
- Betriebsrat (Member)
- Universitätsgewerkschaft wissenschaftliches Personal, Bundesvertretung 13 der GÖD (Vice Chair)
- Verhandlungsteam der GÖD für den Universitätskollektivvertrag (Member)

Christian Teichert
- Institute of Physics: Vice Chair since 2013
- Curriculum Kommission „Werkstoffwissenschaften“ (Member)
- Curriculumskommission Kunststofftechnik (Substitute Member)
- Berufungskommission Materialphysik 2013-2014 (Member)

Markus Kratzer
- Betriebsrat (Member)
- Habilitationskommission Grießer (Member):2014

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

Oskar Paris

Boards and Memberships

- Editorial board member of Scientific Reports, Nature Publishing Group (2012-2015).
- 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).
- Delegate of the Delegate Assembly of the Austrian Science Foundation (FWF) (2011-2015); Vice-Delegate (2015-2019).
- Member of the Commission for International Large Scale Research of the Austrian Academy of Sciences (since 2014)
- Chairman of the Neutrons and Synchrotron Radiation division (NESY) of the Austrian Physical Society (ÖPG) (2012-2014); Vice-chairman (2015).
- Member of the Scientific Advisory Board „Freiburger Zentrum für interaktive Werkstoffe und Bioinspirierte Technologien“ (since 2015)
- 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 large scale European Synchrotron and Neutron facilities: ESRF Grenoble (2012-2014), FRM II, Munich (since 2010)
- 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)
- Member of the Austrian Physical Society

- Reviewer für Optical Materials, Chinese Optics Letters
- 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

- Since 2013 Chair of the Nanometer Structure Devision, IUVSTA
- Since 2013 Board Member, Austrian Physical Society.
- Referee for ÖAD, Czech, Polish and German Science Foundations, Referee for Professorships (France, Netherlands, USA), Ph D Referee (TU Graz,)
- Reviewer for Nature, Science, PRL, PRB, APL, ACS NANO etc.
- 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

- Reviewer ACS Applied Materials & Interfaces, RSC Catalysis, Vacuum, Journal of Chemical Physics, Surface & Coatings Technology, Journal of Materials Science, Nanoscale
- Juror AYPT (Austrian Young Physisists Tournament).

Rainer T. Lechner

- National Delegate for the European Synchrotron User Organisation (ESUO)
- Reviewer for Acta Materialia and Journal of Vacuum Science and Technology B
- Member of the Austrian Physical Society and the Neutrons and Synchrotron Radiation division (NESY)
- Juror AYPT (Austrian Young Physisists Tournament).

13. Picture Gallery

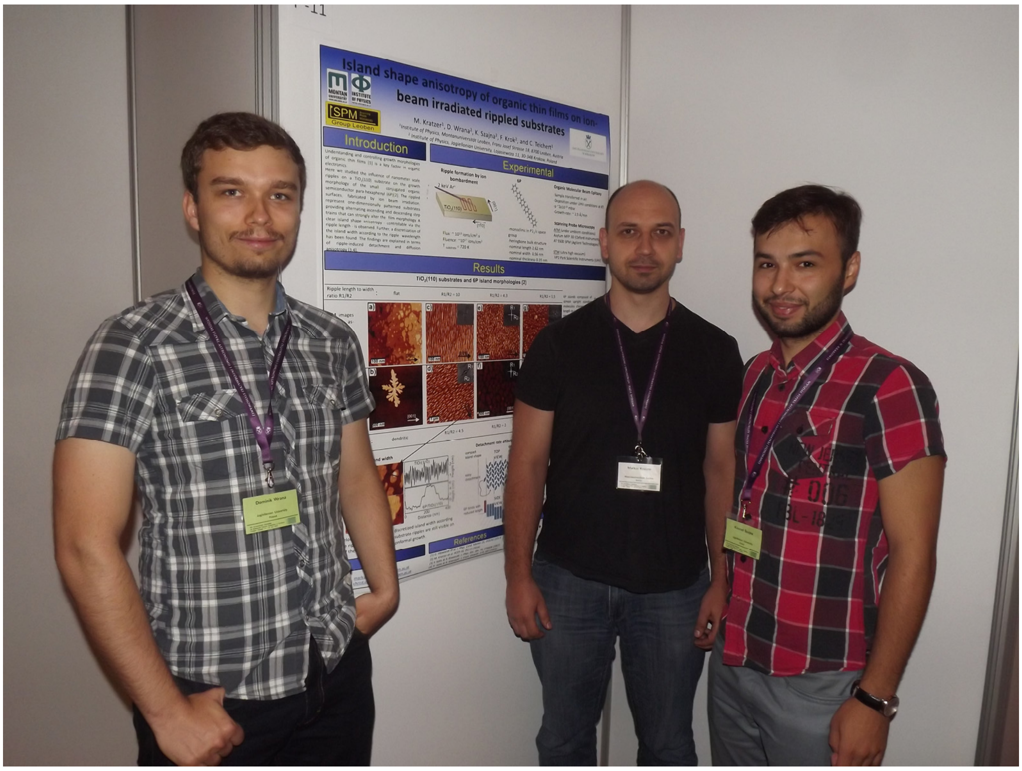
Student Price oft he Austrian Physical Society (ÖPG-Studierenden-Preis) for **Dipl.-Ing. Christian Prehal** for his diploma thesis „In-situ SAXS study on the ion dynamics in microporous carbon based supercapacitors“. From left to right: DI Christian Prehal, Supervisor Univ.-Prof. Dr. Oskar Paris, ÖPG-President Univ.-Prof. Dr. Wolfgang Ernst.

Rektor-Platzer-Ring for **Dip.-Ing. Christian Prehal**, Akademische Feier Montanuniversitaet Leoben

Markus Hartmann (left) and **Soran Nabavi**, proudly showing their New Journal of Physics Highlight certificate.

Markus Kratzer (left) and **Christian Teichert** showing their cover page image from Applied Physics Letters in front of the hot-wall epitaxy apparatus where the samples for the paper were grown.

Lisa Weniger: Dr.Hans Riegel-Fachpreis 2015 by the Kaiserschildstiftung 3rd Rank for a “Vorwissenschatliche Arbeit” based on her experimental work on graphene. in the Scanning Probe Microscopy Group of the institute.



Markus Kratzer: “Best Poster Prize” 8th International Workshop on Nanoscale Pattern Formation at Surfaces, Krakow, Poland, 12.-16.07.2015. **M. Kratzer** (middle) with two interested conference attendees.

Festveranstaltung "30 Jahre Werkstoffe der Elektronik (WdE)".

Top: Three generations of Professors at the Institute of Physics: G. Bauer (3), F. Kuchar (6) and O. Paris (4), together with interim Chair F. Sturm (1), F. Jeglitsch (2), and Rector W. Eichlseder (5). Numbers indicate the position from the left.

Bottom: some of the University teachers in WdE of the last 30 years: From left: Kratzer, Kuchar, Ganitzer, Lutz, Oswald, Lechner, Teichert, Kasper, Bauer, Paris, Noll, Clemens, Sitte, Krenn, Brunner, Meisels.

Kolloquium zu den Nobelpreisen 2014 aus Physik und Chemie an der Montanuniversität. The organizers with the two speakers Henning Riechert (Physics) and Thomas Klar (Chemistry); from left: Sitte, Klar, Wegscheider, Riechert, Teichert, Rector Eichlseder, Paris

Kolloquium zu den Nobelpreisen 2015 aus Physik und Chemie an der Montanuniversität. The organizers with the two speakers Thomas Schwetz-Mangold (Physics) and Kai-Uwe Fröhlich (Chemistry); from left: Sitte, Wegscheider, Fröhlich, Paris Schwetz-Mangold, Teichert

Physicists making delicious ice with liquid nitrogen in the social room of the Institute of Physics on the occasion of R.T. Lechners birthday

Farewell Magdalena Ottrin after 24 years at the Institute of Physics (December 2015).

Institute excursion to ELETTRA synchrotron radiation source in Trieste (June 2014)

Rigorosum Nabavi (November 2014); from left: R. Weinkamer (examiner), S. Nabavi, R. Danzer (rigorosum chair), O. Paris (examiner)

Poster Session: 18th International Winterschool on New Developments in Solid State Physics, Mauterndorf, Austria, 23.-28.2.2014

73rd IUVSTA Workshop “Nanostructures on two-dimensional solids”, 22. – 26.9. 2014, Eisenerz, Austria

9th European NESY Winter-School & Symposium on Neutrons and Synchrotron Radiation including topical highlight lectures on Neutron and Synchrotron Radiation for Industrial Applications, Altaussee (Austria), March 9-13, 2015, Austria

Back cover image: GISAXS pattern from ordered mesoporous thin silica films on silicon substrate

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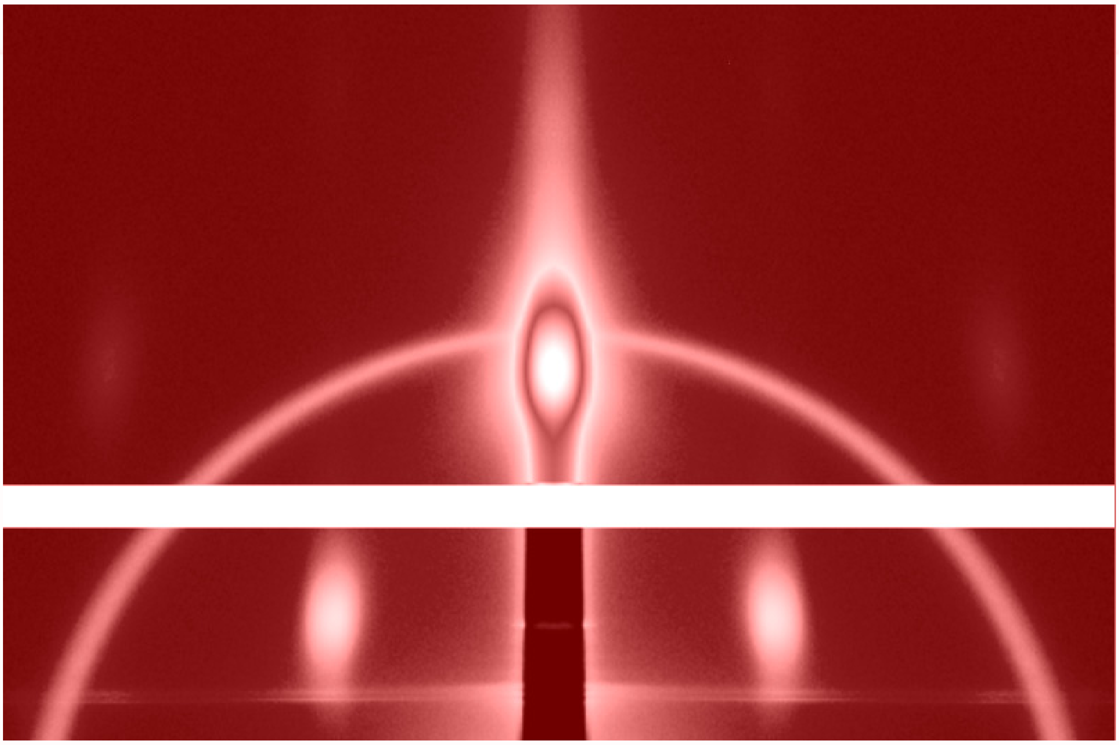

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