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Fachverband Mikrosonden (MI)

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Overview of Invited Talks and Sessions

(Lecture rooms: HSZ 201, MER 02, and MOL 213; Posters: P4)

Invited Tutorial Talks

MI 1.1	Sun	16:00–16:45	HSZ 201	**Positrons probing matter: What we learn about lattice defects and electronic structure using positron beams** — •Christoph Hugenschmidt
MI 1.2	Sun	16:45–17:30	HSZ 201	**Theoretical electron and electron-positron momentum densities of transition metals and their compounds in the presence of many-body correlation effects** — •Liviu Chioncel
MI 1.3	Sun	17:30–18:15	HSZ 201	**Positron annihilation studies at an electron accelerator: From thin films to bulk samples and 3-D imaging** — •Andreas Wagner

Invited Talks of the Joint Symposium "Crystallography in Materials Science" (SYCM)

See SYCM for the full program of the symposium.

SYCM 1.1	Mon	15:00–15:30	HSZ 02	**Complexity on Compression: The Crystallography of High-Density Matter** — •Malcolm McMahon
SYCM 1.2	Mon	15:30–16:00	HSZ 02	**X-Ray Microscopy with Coherent Radiation: Beyond the Spatial Resolution of Conventional X-Ray Microscopy** — •Christian G. Schroer
SYCM 1.3	Mon	16:00–16:30	HSZ 02	**Modulated martensite: A scale bridging Lego game for crystallographers and physicists** — •Sebastian Fähler
SYCM 1.4	Mon	16:45–17:15	HSZ 02	**Switching of magnetic domains reveals evidence for spatially inhomogeneous superconductivity** — •Michel Kenzelmann
SYCM 1.5	Mon	17:15–17:45	HSZ 02	**The key role of magnetic neutron diffraction in materials science** — •Laurent C. Chapon

Invited Talks

MI 2.1	Mon	10:00–10:45	MER 02	**Positronenstrahl-Mikroanalyse - Möglichkeiten und Herausforderungen** — •Torsten E.M. Staab, Matz Haaks, Karl Maier
MI 3.1	Tue	9:30–10:00	MER 02	***In situ* transmission electron microscopy studies of one-dimensional materials** — •Vadim Migunov, Zi-An Li, Spasova Marina, Michael Farle, Rafal E. Dunin-Borkowski
MI 9.1	Thu	9:30–10:00	MER 02	**The martensitic transformation in Co-Ni-Al F-SMA** — •Jaromír Kopeček, Karel Jurek, Michal Landa, Oleg Heczko

Invited Talks of the Joint Focus Session with Accelerator Physics - Beschleunigerphysik (BE)

MI 7.1	Wed	15:00–15:30	MOL 213	**Short-Pulse Operation of Synchrotron Radiation Sources** — •Anke-Susanne Müller
MI 7.2	Wed	15:30–16:00	MOL 213	**Progress in White Beam Diffraction Imaging** — •Andreas Danilewsky

MI 7.3	Wed	16:00–16:30	MOL 213	**Short pulses @ SOLEIL: Femto-Slicing and Low-Alpha** — •Marie Labat
MI 7.4	Wed	16:30–17:00	MOL 213	**Nanomagnets and artificial multiferroics studied with X-ray photoemission electron microscopy** — •Frithjof Nolting

Invited Talks of the Joint Session with KR

MI 11.1	Thu	15:00–15:30	CHE 184	**Crystals: Structure, Properties and Heart of Energy Conversion Devices** — •Tilmann Leisegang, Juliane Hanzig, Erik Mehner, Matthias Zschornak, Falk Meutzner, Tina Nestler, Bianca Störr, Charaf Cherkouk, Ulrike Wunderwald, Dirk C. Meyer

Sessions

MI 1.1–1.3	Sun	16:00–18:15	HSZ 201	**Festkörpercharakterisierung mit Positronen**
MI 2.1–2.9	Mon	10:00–13:00	MER 02	**Untersuchung von kondensierter Materie mittels Positronen-Annihilation**
MI 3.1–3.4	Tue	9:30–11:00	MER 02	**Analytical Transmission Electron Microscopy and Atom Probe Tomography**
MI 4.1–4.3	Tue	11:15–12:00	MER 02	**Scanning Probe Microscopy**
MI 5.1–5.3	Wed	9:30–10:45	MER 02	**Ion Beam Methods**
MI 6.1–6.4	Wed	11:00–12:00	MER 02	**X-ray Imaging, Holography and Tomography**
MI 7.1–7.5	Wed	15:00–17:15	MOL 213	**Synchrotron Radiation (Focus Session with Accelerator Physics)**
MI 8.1–8.10	Wed	17:00–19:30	P4	**Poster: Microanalysis and Microscopy**
MI 9.1–9.5	Thu	9:30–11:00	MER 02	**Functional Materials - Analysis with EBSD, X-Ray Kossel Diffraction and Related Methods (MI jointly with KR)**
MI 10.1–10.3	Thu	11:00–11:45	CHE 184	**Crystallography in Nanoscience (KR jointly with MI)**
MI 11.1–11.8	Thu	15:00–17:30	CHE 184	**Crystallography in Materials Science (KR jointly with DF, MI)**

Mitgliederversammlung des Fachverbandes Mikrosonden

Montag 18:15 MER 02

- Bericht des Fachverbandsvorsitzenden
- Planung der DPG-Tagung 2015
- Verschiedenes

MI 1: Festkörpercharakterisierung mit Positronen

Die Positronenannihilation hat sich seit einigen Jahrzehnten als Methode zur Untersuchung der Real- und Elektronenstruktur von kristallinen Festkörpern bewährt. Positronen, die in Strukturdefekten eingefangen werden (Leerstellen, Leerstellencluster, Versetzungen, Korngrenzen, Ausscheidungen) ändern ihre Annihilationsparameter, so dass Aussagen zur Art und Dichte der Defekte getroffen werden können. In den letzten Jahren ist eine weitere Anwendung in dielektrischen Stoffen hinzugekommen: hier bildet sich Positronium, dessen Lebensdauer ein Maß für das offene Volumen in der Probe ist. So kann bspw. das Volumen zwischen Polymerketten oder Porengrößen in Mikro- und Mesoporen charakterisiert werden. In den drei Tutorial-Vorträgen werden diese Aspekte näher erläutert. Weiterhin werden die beiden Nutzeranlagen für alle Aspekte der Positronenannihilation am FRM-II und an ELBE (HZDR) detailliert vorgestellt. Es wird erläutert, wie man als externer Nutzer Strahlzeit erhalten kann.

Chair: R. Krause-Rehberg (Martin-Luther-Universität Halle-Wittenberg)

Time: Sunday 16:00–18:15 Location: HSZ 201

Tutorial MI 1.1 Sun 16:00 HSZ 201

Positrons probing matter: What we learn about lattice defects and electronic structure using positron beams — •Christoph Hugenschmidt — E21 Physik-Department und FRM II, Technische Universität München, Lichtenbergstraße 1, 85747 Garching

Monoenergetic positrons beams are applied in a large variety of experiments in solid state physics and material science. Examples are spatially resolved defect maps of plastically deformed or irradiated metals, non-destructive investigation of layered systems, the annealing behaviour of defects or the free volume in polymers. At the surface, the annihilation of positrons with core electrons initiates the emission of Auger-electrons that allows the examination of the topmost atomic layer. In addition, the electronic structure such as anisotropies of the Fermi surface can be studied too.

Within this contribution the basic properties of positron annihilation studies will be explained. The benefit of positron beam experiments will be elucidated by selected experiments, such as (i) defect sensitive positron lifetime experiments, (ii) elemental selective (coincident) Doppler broadening spectroscopy of the annihilation line, (iii) angular correlation of annihilation radiation experiments, and (iv) time-dependent positron annihilation induced Auger-electron spectroscopy.

The neutron induced positron source NEPOMUC provides the world's highest intensity of more than 10^9 moderated positrons per second. An overview of the NEPOMUC beam facility and the positron instrumentation is given and future developments and applications of the high-intensity positron beam will be discussed.

Tutorial MI 1.2 Sun 16:45 HSZ 201

Theoretical electron and electron-positron momentum densities of transition metals and their compounds in the presence of many-body correlation effects — •Liviu Chioncel — Theoretische Physik III, Zentrum für Elektronische Korrelationen und Magnetismus Institut für Physik Universität Augsburg — Augsburg Center for Innovative Technology

Valuable information about the nature of many-electron interactions in transition metals and their compounds is obtained from experiments based on Compton and positron annihilation spectroscopy the later especially in the form of angular correlation of annihilation radiation measurements. These experiments access the electron momentum density and the momentum density of annihilating electron-positron pairs. Here we review theoretical state of the art techniques that combine Density Functional and Dynamical Mean Field Theory which allows to calculate the electron momentum densities. We survey recent experiments and calculations for paramagnetic and ferromagnetic transition metals and half-metallic ferromagnets.

Tutorial MI 1.3 Sun 17:30 HSZ 201

Positron annihilation studies at an electron accelerator: From thin films to bulk samples and 3-D imaging — •Andreas Wagner — Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstr. 400, 01328 Dresden, Germany

Positron annihilation lifetime spectroscopy serves as a perfect tool for studies of open-volume defects in solid materials such as vacancies, vacancy agglomerates, and dislocations. Moreover, structures in porous media can be investigated ranging from 0.3 nm to 30 nm employing the variation of the positronium lifetime with the pore size. While lifetime measurements close to the material's surface can be performed at positron-beam installations, bulk materials, fluids, gases, bio-materials or composite structures cannot or only destructively accessed by positron beams. In the tutorial, a set of new installations at the superconducting electron linear accelerator ELBE will be discussed. Key to all experiments is the timing resolution and the variability in pulse repetition rate which enables new ways of materials research with positrons. Depth dependent defect studies (both annihilation lifetime and Doppler-broadening) on thin films are enabled by a tunable monoenergetic positron beam. Experiments using high-energy electron-bremsstrahlung as a source for pair production inside the investigated samples release vacuum constraints and allow studying structural defects on the atomic scale even for radioactive samples with significant intrinsic activities. Some recent examples and results will be given and a facility extension for in-situ defect generation studies will be presented.

MI 2: Untersuchung von kondensierter Materie mittels Positronen-Annihilation

Chair: R. Krause-Rehberg (Martin-Luther-Universität Halle-Wittenberg)

Time: Monday 10:00–13:00 Location: MER 02

Invited Talk MI 2.1 Mon 10:00 MER 02

Positronenstrahl-Mikroanalyse - Möglichkeiten und Herausforderungen — •Torsten E.M. Staab[1], Matz Haaks[2,3] und Karl Maier[2] — [1]LCTM, Universität Würzburg, Röntgenring 11, D-97070 Würzburg, Germany — [2]HISKP, Universität Bonn, Nußallee 14-16, D-53115 Bonn, Germany — [3]Aero-Laser GmbH, Unterfeldstr. 12, D-82467 Garmisch Partenkirchen

Während eine Elektronenstrahl-Mikrosonde die 2-dimensionale Abbildung der Verteilung von Elementen im Mikrometerbereich mittels deren charakteristischer Röntgenstrahlung ermöglicht, kann eine entsprechende 2-dimensionale Abbildung von leerstellenartigen Gitterbaufehlern durch eine Positronenstrahl-Mikrosonde erfolgen, da Positronen sensitiv auf Leerstellen und leerstellenartige Gitterbaufehler in Festkörpern sind. Dabei können nicht nur Leerstellen an sich sondern auch deren atomare Umgebung charakterisiert werden.

Neben verschiedenen Anwendungsmöglichkeiten der Positronenstrahl-Mikrosonde – eines modifizierten Rasterelektronenmikroskops – werden Beispiele zur Messung und zur Identifikation von Fehlstellen in Halbleitern und Aluminiumlegierungen mit Positronen gezeigt. Kombiniert mit anderen Methoden wie der Röntgenabsoptionsspektroskopie (XAFS) und der Röntgenkleinwinkelstreuung (SAXS), ergibt sich ein komplementäres Bild des Wechelspiels von Leerstellen und Legierungsatomen in Aluminiumlegierungen. Mit ab-initio Rechnungen ermittelte Atompositionen um Gitterbaufehler dienen dazu, Spektren zu simulieren, die dann direkt mit experimentellen Daten verglichen werden.

MI 2.2 Mon 10:45 MER 02

Development of a time- and position-resolving detector for 4D-AMOC — •Ulrich Ackermann, Werner Egger, Peter Sperr, Andreas Bergmaier, Christoph Greubel, and Günther Dollinger — Universität der Bundeswehr München, Institut für angewandte Physik und Messtechnik, Werner-Heisenberg-Weg 39, 85577 Neubiberg

The Pulsed Low Energy Positron System (PLEPS) at NEPOMUC at the Munich research reactor FRM2 is a powerful tool for depth resolved investigations of defects in solids via positron annihilation lifetime spectroscopy (PALS). Besides PALS two dimensional Age Momentum Correlation Measurements (2D-AMOC) are also possible where one measures the longitudinal momentum of the electron annihilating with the positron in addition with the positrons lifetime.

To measure the positrons lifetime together with the entire 3D-momentum of the electron annihilating with the positron (4D-AMOC) a pixelated Germanium detector in coincidence with a position sensitive scintillation detector will be used. The constraints for the scintillation detector are about 100 ps time resolution (FWHM) and circa 2 mm spatial resolution (FWHM) over an area of 12 cm^2 at gamma energies of 511 keV, respectively.

As scintillation detector we intend to use a MCP image intensifier detector coupled to a scintillator in addition with VME and NIM electronic modules and a MARaBOU/ROOT based data acquisition. First results of time resolution and position resolution with the scintillation detector setting will be presented.

MI 2.3 Mon 11:00 MER 02

Implementing the Munich Scanning Positron Microscope at NEPOMUC — •Marcel Dickmann[1], Christian Piochacz[2,3], Werner Egger[1], Gottfried Kögel[1], Peter Sperr[1], Christoph Hugenschmidt[2,3], and Günther Dollinger[1] — [1]Universität der Bundeswehr München, LRT2, D-85577 Neubiberg, Germany — [2]Technische Universität München, Physik Department E21, D-85748 Garching, Germany — [3]FRM2, Technische Universität München, D-85748 Garching, Germany

Positron annihilation lifetime spectroscopy is a very sensitive method to analyze non-destructively small open volume defects, e.g. vacancies, vacancy clusters, and dislocations. Defect-types and their concentrations can be determined. The Munich Scanning Positron Microscope (SPM) generates a focused, pulsed low-energy positron beam for positron lifetime measurements with a high lateral resolution ≥ 1 μm. By varying the beam energy, depth resolutions in the sub-μm range can be obtained, which makes 3D defect microscopy possible. With the SPM defect distributions close to crack surfaces have been successfully studied in pure copper and in the alloy Al 6013. The main limitation in these studies was the low count-rate obtainable with conventional laboratory positron sources, which leads to exceedingly long measurement times. Therefore, to increase the beam intensity, the SPM is transferred to the high intense positron source NEPOMUC at the FRM II research reactor in Munich. To match the stringent requirements on positron beam brilliance of the SPM, an interface, that increases the phase space density of the NEPOMUC beam, was built, and successfully tested.

MI 2.4 Mon 11:15 MER 02

Spin polarized 2D-ACAR study of the electronic structure of Nickel — •Hubert Ceeh[1], Josef-Andreas Weber[1], Michael Leitner[1], Christoph Hugenschmidt[1], Liviu Chioncel[2], Diana Benea[3], and Peter Böni[1] — [1]Technische Universität München, Physik Department, Lehrstuhl E21, James-Franck-Straße, D-85748 Garching, Germany — [2]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [3]Chemistry Department, University Munich, Butenandstraße 5-13, D-81377 München, Germany

2D-ACAR (Angular Correlation of Positron Annihilation Radiation) is a well known technique for the investigation of the electronic structure, i.e the Fermi surface of a material. For the properties of a metal the Fermi surface is a most important characteristic as it defines the boundary between occupied and unoccupied states in reciprocal space. In this contribution we give an overview on the measurement principle of spin-polarized 2D-ACAR. We then present our measurement of the momentum-density distributions of magnetic electrons in Nickel and compare these results with recent theoretical calculations based on the combined density functional and dynamical mean field theory. The overall structure of the experimental momentum densities are already reasonably reproduced without including dynamical electronic correlations, however we show that the slight quantitative discrepancies are reduced including the electronic correlations.

15 min. break

MI 2.5 Mon 11:45 MER 02

Positronen-Annihilations-Spektroskopie mit gepixelten Germaniumdetektoren zur 3D-Messung des Elektronenimpulses — •Benjamin Löwe[1], Markus Reiner[2], Werner Egger[1], Christoph Hugenschmidt[2] und Günther Dollinger[1] — [1]Universität der Bundeswehr, LRT2, Werner-Heisenberg-Weg 39, 85577 Neubiberg, Germany — [2]FRM II, Technische Universität München, Lichtenbergstraße 1, 85747 Garching, Germany

Aus dem dopplerverbreiterten Annihilationsspektrum von Positronen in Materie, kann man Aussagen über die chemische Umgebung des Annihilationsortes erhalten. Bei der Coincident Doppler Broadening Spectroscopy wird die Energie der Annihilationsstrahlung mit zwei Germaniumdetektoren in Koinzidenz gemessen. Dadurch erhält man eine Projektion des Elektronenimpulses. Um den vollen Elektronenimpuls zu messen ist es notwendig, zusätzlich zur Energie, die Winkelkorrelation der beiden Annihilationsquanten aufzunehmen.

Um dies zu erreichen haben wir ein Detektorsystem bestehend aus zwei 36-fach gepixelten Germaniumdetektoren sowie einer digitaler Datenaufnahme aufgebaut. An einem intensiven Positronenstrahl wurden bereits erste Testmessungen durchgeführt, die in diesem Beitrag vorgestellt werden.

MI 2.6 Mon 12:00 MER 02

Apparatus for In-situ Defect Analysis (AIDA) — •Maciej Oskar Liedke[1], Wolfgang Anwand[1], Kay Potzger[2], Alireza Heidarian[2], Rantej Bali[2], and Andreas Wagner[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Radiation Physics, Bautzner Landstraße 400, 01328 Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstraße 400, 01328 Dresden, Germany

A unique high vacuum system combining material evaporation and ion beam modification with positron annihilation spectroscopy (PAS) has been developed and installed in the Helmholtz-Zentrum Dresden-

Rossendorf. The in-situ system is capable to perform Doppler broadening spectroscopy as well as resistometry (4 point probe). It is an end station of the Slow-Positron System of Rossendorf (SPONSOR) that provides a mono-energetic positron beam pre-accelerated in the range of 80 eV to 35 keV thus enabling sample depth profiling. The main focus of studies is the in-situ modification (during growth, ion irradiation, cooling/annealing) and the analysis of open volume defects and the chemical environment in thin films of, e.g., memristive oxides or metal alloys. First results on the FeAl ion irradiation/annealing driven magnetic phase transition between the paramagnetic and ferromagnetic state as a function of the open volume defects will be shown. The project is financed by the Impuls- und Vernetzungsfonds of the Helmholtz Association (code VH-VI-442).

MI 2.7 Mon 12:15 MER 02

Ion implantation induced damage in ZrO_2 probed by a slow positron beam — Wolfgang Anwand[1], Xin Ou[2], Maik Butterling[1], and •Andreas Wagner[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Radiation Physics, POB 51 01 19, 01314 Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, POB 51 01 19, 01314 Dresden, Germany

ZrO_2 in a cubic phase is generally known as YSZ (yttria-stabilized zirconia). YSZ is a promising material which exhibits excellent radiation resistance and chemical stability. It can be applied e.g. for the inter-matrix layer of fuel cells or for covering and storage of nuclear waste. The effect of irradiation on YSZ has already been intensively investigated via single ion beam implantation. Most of the experimental work was performed in order to simulate the radiation damage from alpha particles by He+ implantation, or to simulate the neutron radiation damage as well as the damage introduced from alpha recoils by implantation of heavy ions. Both I ions and He ions were implanted into YSZ samples. Single implantation of I ions as well as He ions, implantation of both types of ions at different sequence, and a simultaneous implantation with a dual beam were carried out in order to create varying defect profiles. Thereby it was intended to distinguish the various influences of the heavy and light ions on the defect profiles and to clarify a possible He retention or release after implantation. The implantation-induced damage was investigated by a mono-energetic slow positron beam.

MI 2.8 Mon 12:30 MER 02

Long-term ageing effects in reactor pressure vessel steels investigated by positron annihilation spectroscopy — •Maik Butterling[1], Wolfgang Anwand[1], Frank Bergner[2], Andreas Ulbricht[2], Andreas Wagner[1], and Arne Wagner[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Radiation Physics, POB 51 01 19, 01314 Dresden, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, POB 51 01 19, 01314 Dresden, Germany

Neutron irradiation of reactor pressure vessel steels leads to the formation of nano-sized defects which can deteriorate the material. An understanding of the microstructural evolution of the material is important for making reliable security assessments about possible future long-term operation of nuclear power plants.

So-called late-blooming phases [1-3] are formed after long-term irradiation and lead to considerable material ageing effects. Encouraging factors for the formation of these phases are a low Cu-content, moderate to high contents of Mn and Ni, low irradiation temperatures and different neutron fluxes.

Positron annihilation lifetime spectroscopy which is ideally suited for the detection and characterization of these irradiation-induced defects was applied for different selected materials which fulfill these conditions in order to investigate the occurrence and behavior of these phases.

[1] G.R. Odette, Mater. Res. Soc. Symp. Proc. 373 (1995) 137-148
[2] G.R. Odette and B.D. Wirth, J. Nucl. Mater. 251 (1997) 157
[3] R. Ngaymam-Happy et al., J. Nucl. Mater. 426 (2012) 198-207

MI 2.9 Mon 12:45 MER 02

MnSi Single Crystal Growth - Effects of the Outgasing of Mn Studied by Positron Annihilation Spectroscopy — •Markus Reiner[1,2], Wolfgang Anwand[3], Andreas Bauer[1], Maik Butterling[3], Thomas Gigl[1,2], Christian Pfleiderer[1], Andreas Wagner[3], and Christoph Hugenschmidt[1,2] — [1]Technische Univeristät München, Physik-Department, Lehrstuhl E21, James-Franck-Straße 1, 85748 Garching — [2]Technische Univeristät München, ZWE FRM-II, Lichtenbergstraße 1, 85748 Garching — [3]Helmholtz-Zentrum Dresden-Rossendorf, Kernphysik, Bautzner Landstraße 400, 01328 Dresden

The intermetallic B20 compound MnSi exhibits outstanding magnetic properties. Both the understanding of complex magnetic phenomena and the possible application as extremely efficient data storage material in future devices require the production of defect-free single crystalline MnSi.

For the present study, several MnSi single crystals have been grown from initial rods with a varying Mn excess in order to compensate the outgasing of Mn during crystal growth. The quality of the various crystals was examined by (coincident) Doppler broadening and positron lifetime spectroscopy. Wafers were investigated with the highly intense positron beam NEPOMUC at the FRM-II. In addition, the whole crystal rods were examined at the GIPS facility in the HZDR

The results clearly show that the open volume defects in MnSi can be efficiently reduced by inducing a slight Mn excess of several atomic percent in the initial rods used for single crystal growth.

MI 3: Analytical Transmission Electron Microscopy and Atom Probe Tomography

Chair: Hartmut S. Leipner (Martin-Luther-Universität Halle-Wittenberg)

Time: Tuesday 9:30–11:00 Location: MER 02

Invited Talk MI 3.1 Tue 9:30 MER 02

***In situ* transmission electron microscopy studies of one-dimensional materials** — •Vadim Migunov[1], Zi-An Li[2], Spasova Marina[2], Michael Farle[2], and Rafal E. Dunin-Borkowski[1] — [1]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Peter Gruenberg Institute, Research Centre Juelich, Juelich, Germany — [2]Faculty of Physics and CeNIDE, University of Duisburg-Essen, Duisburg, Germany

As a result of recent progress in *in situ* transmission electron microscopy (TEM), the mechanical, electronic and magnetic properties of nanoscale materials and devices can now be investigated directly and correlated with their local three-dimensional morphologies, atomic structures and chemical compositions.

We have studied the mechanical, electronic and field emission properties of a variety of different nanostructures, including InAs nanowires and CdS nanocomb-like structures, using methods based on scanning probe microscopy (SPM) *in situ* in the TEM. In particular, we have used a combination of SPM and off-axis electron holography in the TEM to measure electrostatic potential and charge density distributions inside and outside materials with nm precision, both in projection and in three dimensions. Such information about local functional properties is important both for fundamental research and for the design of novel nanoscale devices.

The first author gratefully acknowledges the award of a Heinz-Bethge-Nachwuchspreis for part of this work.

MI 3.2 Tue 10:00 MER 02

New Applications in Atom Probe Tomography — •H.-Ulrich Ehrke — CAMECA, München

Atom probe tomography (APT) is known as a method for element and isotope analysis with sub-nm resolution in 3D. Innovations in APT and focused ion beam based sample preparation have enabled new applications including semiconductors and insulating materials.

Variability in metal-oxide-semiconductor (MOS) transistors has substantially increased due to continuous decreasing feature size. APT can provide elemental mapping in MOS transistors, and correlate such electrical performance with dopant concentration, showing that threshold voltage in 65 nm-node n-MOS transistors is positively correlated with the channel dopant concentration.

In geological materials, APT is now providing unique information for understanding the thermal history and mechanisms of mineral reaction, mineral exchange and radiation damage. In zircon crystals,

$^{207}Pb/^{206}Pb$ ratios for nm-scale domains (< 20 000 atoms Pb) average 0.17 ± 0.04 for a 2.4 Ga zircon and 0.43 ± 0.14 for a 4.0 Ga zircon in agreement with the ratios measured by SIMS over much larger volumes (100's μm^3) 0.1684 and 0.4269, respectively).

In metallic glass research, the glass forming ability of high Fe-content glasses for low-cost transformer applications is improved by small copper additions. $Fe_{76-x}C_{7.0}Si_{3.3}B_{5.0}P_{8.7}Cu_{0.7}$ glass phase-separates into α-Fe precipitates, ultrafine spheroidal ϵ-Cu-rich precipitates, silicon-depleted Fe_3(P,B,C), and Fe_3C after thermal annealing for 30 min. at 729K.

MI 3.3 Tue 10:30 MER 02

Stapelfehler als Ursache für Degradation von Si-Solarzellen — •Volker Naumann[1], Dominik Lausch[1], Andreas Graff[2], Jan Bauer[3], Angelika Hähnel[3], Otwin Breitenstein[3], Stephan Grosser[1] und Christian Hagendorf[1] — [1]Fraunhofer-Center für Silizium-Photovoltaik CSP, Halle (Saale) — [2]Fraunhofer-Institut für Werkstoffmechanik IWM, Halle (Saale) — [3]Max-Planck-Institut für Mikrostrukturphysik, Halle (Saale)

In Solarmodulen können bei Reihenschaltung hohe Spannungen gegen Erdpotenzial auftreten. Diese führen bei bestimmten klimatischen Bedingungen zur sogenannten potenzialinduzierten Degradation (PID), was mit teils dramatischen Leistungsverlusten der betroffenen Solarmodule durch Kurzschließen der kristallinen Si-Solarzellen einher geht.

Die physikalische Ursache der Kurzschlüsse wird mit elektronenmikroskopischen Methoden untersucht. Zum Auffinden der Defekte wurde REM/EBIC angewendet. An mittels FIB erzeugten Querschnitten sind die PID-Kurzschlussdefekte mit EBIC als zweidimensionale Defekte in {111}-Ebenen erkennbar. TEM-Untersuchungen ergeben, dass es sich bei den Defekten um Stapelfehler handelt. Mit STEM/EDX lässt sich eine Dekoration der Stapelfehler mit Na nachweisen. Die Dichte von Na in der Stapelfehlerebene wurde zu 10^{14} bis 10^{15} Atome pro cm^2 bestimmt. Es wird vermutet, dass Natriumatome in Stapelfehlern eine große Dichte elektronischer Zustände erzeugen. Die Kurzschlüsse, die bei PID entstehen, werden folglich darauf zurückgeführt, dass die Stapelfehler im Siliziumkristall durch das Eindringen von Na elektrisch leitend werden und den pn-Übergang kurzschließen.

MI 3.4 Tue 10:45 MER 02

Microstructural Investigation of Recombination Active Defects in Multicrystalline Silicon Solar Cells — •Dominik Lausch[1], Angelika Hähnel[2], Martina Werner[1], Jan Bauer[2], Otwin Breitenstein[2], and Christian Hagendorf[1] — [1]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany

The focus of this work will be on the microstructural investigation of different types of defects in mc-Si solar cells introduced in a previous publication. It is shown that defect types observed on a macroscopic scale could be directly related to structures on a microscopic scale by using advanced and newly applied microstructural microscopy methods. One defect type could be clearly correlated to iron precipitates located at defect structures of the underlying wafer by TEM analysis. To discuss the physical behaviour at the different defect classes temperature dependent EBIC measurements have been performed. Based on these results a model for the different classified types will be proposed explaining the observed recombination and prebreakdown behavior.The knowledge obtained can be reversibly interconnected to the macroscopic investigation on an industrial level to work on a solution to avoid these problems.

MI 4: Scanning Probe Microscopy

Time: Tuesday 11:15–12:00 Location: MER 02

MI 4.1 Tue 11:15 MER 02

Towards the measurement of atomic-scale forces associated with a superconducting transition — •Angelo Peronio and Franz J. Giessibl — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Universitätsstraße 31, D-93053 Regensburg, Germany

The superconducting phase transition alters the electron energy spectrum of a metal, opening up a gap in the density of electronic states around the Fermi energy. The width of this is gap few meV at most, reflecting the strength of the interaction that binds the electrons in superconducting Cooper pairs. This modification of the electronic spectrum, albeit slight, is sufficient to reduce the friction of a niobium surface by a factor of 3 across the superconducting transition temperature [1].

Driven by this evidence, we will present an attempt to detect atomic-scale forces associated with the superconducting transition. In particular, we investigated a well-defined test system with a qPlus AFM sensor [2] equipped with a niobium tip, in order to map the interaction potential between the tip apex and the sample.

References:

[1] Kisiel et al., Nat. Mater. 10 (2011) 119
http://dx.doi.org/10.1038/nmat2936
[2] Giessibl, Appl. Phys. Lett. 73 (1998) 3956
http://dx.doi.org/10.1063/1.122948

MI 4.2 Tue 11:30 MER 02

Ultrasound plus Heterodyne Detection enables SubSurface sensitivity in an AFM — •Gerard J. Verbiest[1] and Marcel J. Rost[2] — [1]JARA- FIT and II. Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]Kamerlingh Onnes Laboratory, Leiden University, P.O. Box 9504, 2300 RA Leiden, The Netherlands

Similar to the sonar of a submarine, it is possible to reach subsurface sensitivity with an AFM: it has been demonstrated that 20 nm small nanoparticles can be resolved, even if they are buried 500 nm deep in a sample. To enable this, Heterodyne Force Microscopy uses two ultrasonic signals in the order of a few MHz, which are sent through the cantilever and the sample, respectively. To detect the sample vibration, the ultrasonic frequencies are chosen slightly different to generate a low-frequency heterodyne force via the nonlinear interaction between the cantilever's tip and the sample. It is this heterodyne signal that contains the subsurface information. However, how this signal is exactly generated is not known.

We developed a general analytical model [1] to quantitatively explain the generation of the heterodyne signal. Standard textbook equations fail in this case, as they are all based on second order approximations. We confirm our results with both an experiment [2] and a full numerical calculation [3] on the example of Heterodyne Force Microscopy.

[1] G.J. Verbiest, and M.J. Rost, Nature Physics submitted
[2] G.J. Verbiest et al., Nanotechnology 24, 365701 (2013)
[3] G.J. Verbiest et al., Ultramicroscopy 135, 113 (2013)

MI 4.3 Tue 11:45 MER 02

Quantum-Emitter Fluorescence Lifetime Imaging Using a Single NV Center — •Andreas W. Schell[1], Philip Engel[1], Julia F. M. Werra[2], Christian Wolff[3], Kurt Busch[2,3], and Oliver Besnon[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, AG Nanooptik, D-12489 Berlin, Germany — [2]Humboldt-Universität zu Berlin, Institut für Physik, AG Theoretische Optik & Photonik, D-12 D-12489 Berlin, Germany — [3]Max-Born-Institut, D-12 D-12489 Berlin, Germany

Knowledge about the local density of optical states (LDOS) is a key requirement for understanding and engineering the coupling of emitters to photonic and plasmonic structures. One way to gain this knowledge is to use atomic force microscope nanomanipulation techniques to control the coupling of a single nitrogen vacancy (NV) center in nanodiamond to the structures of interest and use its varying decay rate as a measure for the LDOS [1].

Here, we will show a more sophisticated approach which uses an NV centers as a scanning probe. With a nanodiamond containing a single NV center glued to the tip of an atomic force microscope the LDOS is mapped out in a very controlled way in all three dimensions, giving insight into the local behavior of the coupling [2]. By comparison with three-dimensional ab-initio simulation this enables for quantitative understanding of local electromagnetic effects on the nanoscale.

[1] A. W. Schell et. al., Optics Express 19, 8, 7914 (2011).
[2] A. W. Schell et. al., submitted (2013).

MI 5: Ion Beam Methods

Chair: Enrico Langer (TU Dresden)

Time: Wednesday 9:30–10:45 Location: MER 02

MI 5.1 Wed 9:30 MER 02

Materials Analysis with Electron Beam Ion Sources — J. König[1], L. Bischoff[3], U. Kentsch[2], M. Kreller[1], W. Pilz[3], E. Ritter[1], M. Schmidt[1], A. Silze[1], and •G. Zschornack[2] — [1]DREEBIT GmbH, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Electron beam ion sources (EBIS) are able to create a spectrum from low to highly charged ions from gaseous, liquid, or solid primary materials. The high density electron beam in an ultra-high vacuum environment inside of these sources ionizes the material under very well controllable operation parameters. Thus, an ion beam with a sharp energy distribution to be set between some 100 eV and several 10 keV is formed. This allows for a precise analysis of the material components with a relative sensitivity for abundances down to 10^{-4} and a relative mass resolution on the order of 10^{-3}, accurate enough to distinguish between isotopes or molecular ions with small mass differences. In this presentation, we give an overview of materials analysis techniques using easy-to-handle tabletop-sized electron beam ion sources of the Dresden EBIS type. Mass spectrometry measurements with ion sources in combination with bending magnets or ExB filters for mass-to-charge ratio analysis are presented. Furthermore, in comparison to analysis methods where sample material is introduced directly into the source, results from secondary ion mass spectrometry with standard as well as focused ion beam (FIB) EBIS setups are shown. Finally, applications for the presented methods will be discussed.

MI 5.2 Wed 10:00 MER 02

Helium and Neon Ion Microscopy. Extending the frontiers of nanotechnology — •Peter Gnauck, Lars-Oliver Kautschor, and Mohan Ananth — Carl Zeiss Microscopy, Oberkochen, Germany

The Helium Ion Microscope has been described as an impact technology offering new insights into the structure and function of nanomaterials. Combining a high brightness Gas Field Ion Source (GFIS) with unique sample interaction dynamics, the helium ion microscope provides images offering unique contrast and complementary information to existing charged particle imaging instruments such as the SEM and TEM. Formed by a single atom at the emitter tip, the helium probe can be focused to below 0.25nm offering the highest recorded resolution for secondary electron images. The small interaction volume between the helium beam and the sample also results in images with stunning surface detail . Besides imaging, the helium ion beam can be used for fabricating nanostructures at the sub-10nm length scale. The helium ion beam has been used for deposition and etching in conjunction with appropriate chemistries. Helium induced deposition results in higher quality deposits than with Ga-FIB or EBID (Electron Beam Induced Deposition). Finally, the helium ion beam can be used for direct sputtering of different materials. Patterning of graphene has resulted in 5nm wide nanoribbons and 3.5nm holes in silicon nitride membranes have been demonstrated. This work has culminated in the development of an ion microscope with a gas field ion source that can operate with both He and Ne.

MI 5.3 Wed 10:30 MER 02

Depth Profiling of OLED Materials by Cluster Ion Beams. — •Andrey Lyapin[1], John S. Hammond[2], Sankar N. Raman[2], Scott R. Bryan[2], Nicholas C. Erickson[3], and Russell J. Holmes[3] — [1]Physical Electronics GmbH, Fraunhoferstr. 4, D-85737, Ismaning, Germany — [2]Physical Electronics, 18725 Lake Drive East, Chanhassen, MN, 55317, USA — [3]University of Minnesota, Minneapolis, MN, 55455, USA

The improvements in the efficiencies for OLED structures have recently focused on the incorporation of more effective organic materials and the development of novel structures for arranging these organic materials. Multi-layer devices, graded composition devices and novel electrical contact layers to the organic materials are all being rapidly developed. The need for analytical techniques to elucidate the organic thin film structures as a function of device fabrication and lifetime studies is becoming extremely important. The past few years have witnessed a paradigm shift in the use of cluster ion beams for the sputter depth profiling of organic materials in conjunction with the surface analysis techniques. Today the use of low-energy monatomic ion beams such as Ar^+ for depth profiling of a wide range of organic materials, including multi-layer organic thin films and organic light emitting diodes (OLEDs) has been replaced with cluster ions such as $C_{60}{}^+$ and Ar gas cluster ion beams (GCIB). The presentation will illustrated the capability to provide quantitative compositional depth profiling of OLEDs from the XPS depth profile analysis of graded composition multilayer OLED films.

MI 6: X-ray Imaging, Holography and Tomography

Chair: Christian Schroer (TU Dresden)

Time: Wednesday 11:00–12:00 Location: MER 02

MI 6.1 Wed 11:00 MER 02

Phase retrieval in near-field X-ray holography based on separation of object and probe — •Anna-Lena Robisch, Matthias Bartels, and Tim Salditt — Institut für Röntgenphysik, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

X-ray full-field holography offers quantitative amplitude and phase contrast on the nm-scale. However the image quality suffers form imperfections and aberrations in the illuminating beam.

The general way of reducing such unwanted features is to divide the data by the intensity profile of the illumination before performing phase reconstruction which allows to get the real space image of the sample back. This procedure is mathematically not correct; as the division of the complex illumination in amplitude and phase should be performed in real space where the exit wave right behind the sample can be modeled as the product of the sample's transmission function and the incoming beam. One possibility of reconstructing object and probe in the described way is via ptychography[1].

Here we present an algorithm that can be interpreted as a generalization/extension to ptychography using defocus scanning instead of lateral scanning in one fixed plane. Similar to ptychography simultaneous reconstruction of object and probe is possible [2]. Besides the algorithmic concept and simulations first experimental results using data recorded at the nano-scale imaging beamline DESY/PETRAIII/P10 are shown.

[1] P. Thibault et al., ULTRAMICROSCOPY 109, 338-343 (2009)
[2] A-L. Robisch, T. Salditt, OPT EXPRESS 21(20), (2013)

MI 6.2 Wed 11:15 MER 02

High resolution coherent diffractive imaging with a table-top high harmonic source — •Sergey Zayko[1], Eike Mönnich[1], Murat Sivis[1], Tobias Mey[3], Dong-Du Mai[2], Klaus Mann[3], Tim Salditt[2], and Claus Ropers[1] — [1]1IV. Institute of Physics, University of Göttingen, Germany — [2]Institute for X-Ray Physics, University of Göttingen, Germany. — [3]Laser Laboratorium Göttingen, Germany

High harmonic up-conversion of femtosecond laser pulses allows for the generation of coherent extreme ultraviolet radiation from table-top devices. Here, we present a study of coherent diffractive imaging (CDI) using high harmonic generation at a wavelength of 34.7 nm using amplified 800 nm femtosecond laser pulses. The setup employs a toroidal grating monochromator in order to carry out diffraction-limited CDI at a reduced spectral bandwidth. Diffraction images for several lithographically prepared objects were recorded, and successful object reconstructions were obtained by means of iterative phase retrieval algorithms. Resolutions of 38 nm and 34 nm are achieved for a single exposure of 5 s and accumulating multiple exposures, respectively, corresponding to the maximum achievable resolution given by the numerical aperture of the detection setup. Reconstructions for objects up to about 10 micrometres diameter were performed, presently limited by the transverse coherence length of the incident wavefront, which was independently characterized. A further increase of the photon flux and a reduction of the exposure times will be reached by utilizing 400 nm pump pulses, and the spatial resolution will be improved by the use of shorter harmonic wavelengths.

MI 6.3 Wed 11:30 MER 02

Multi-layer Fresnel zone plates towards high resolution soft and hard x-ray microscopy — •Umut Tunca Sanli[1], Kahraman Keskinbora[1], Corinne Grévent[1], Marcel Mayer[1], Adriana V. Szeghalmi[2], Keith Gregorczyk[3], Anna-Lena Robisch[5], Tim Salditt[5], Mato Knez[3,4], and Gisela Schütz[1] — [1]MPI for Intelligent Systems — [2]Friedrich-Schiller-University Jena — [3]CIC nanoGUNE Consolider — [4]IKERBASQUE Basque Foundation for Science — [5]Institut für Röntgenphysik, Universität Göttingen

We fabricate full-material multi-layer Fresnel zone plates (ML-FZPs) by depositing alternating layers of high and low absorbing materials on glass fibers via Atomic Layer Deposition (ALD) followed by a slicing process with a Focused Ion Beam. Depending on their thicknesses the FZPs may be optimized to focus photons in a wide range from soft x-rays to gamma rays. We recently resolved 21 nm structures at 1 keV by direct imaging experiments. For hard x-rays, at 7.9 keV, Fourier analysis of the diffraction patterns gives clues about sub 30 nm resolution. The key to improve the resolution is to increase the Diffraction Efficiency (DE) in order to compensate for the efficiency losses associated with thinner zones. Our newest Al2O3-HfO2 FZPs are theoretically twice as efficient as our previous Al2O3-Ta2O5 FZPs at 1 keV and for dr = 11 nm. According to the coupled wave theory, the DE can be improved by 5 times by using commercially available materials for the ALD, such as Ir-Al2O3. It is expected, that the number of materials available with the ALD will increase allowing further improvement of the FZP performance.

MI 6.4 Wed 11:45 MER 02

High Throughput Fabrication of Fresnel Zone Plates *via* Ion Beam Lithography — •Kahraman Keskinbora, Corinne Grévent, Umut Tunca Sanli, Ulrike Eigenthaler, and Gisela Schütz — Max Planck Institute for Intelligent Systems, 70569, Stuttgart, Germany

Fabrication of high resolution Fresnel Zone Plates (FZPs) by means of e-beam Lithography (EBL) have contributed to the establishment of the X-ray microscopy. However, EBL is an intricate and costly technique. Here, alternatively, we demonstrate the rapid fabrication of FZPs *via* direct write ion beam lithography (IBL) with resolutions approaching those of commercially available EBL-FZPs. Fabrication of 50 μm wide FZP with 50 and 30 nm outermost zone widths were completed in less than 13 and 9 minutes, respectively. Utilizing these IBL-FZBs as the focusing optics in a soft X-ray microscope, it was possible to clearly resolve features of 28 down to 21 nm size with respective cut-off half-pitch resolutions of 24.5 and 21 nm. We believe this rapid fabrication technique will have positive impact on the development of laboratory based soft X-ray microscopy and in applications where large arrays of FZPs are required, such as zone plate array lithography or disposable FZPs for FEL applications.

MI 7: Synchrotron Radiation (Focus Session with Accelerator Physics)

Time: Wednesday 15:00–17:15 Location: MOL 213

Invited Talk MI 7.1 Wed 15:00 MOL 213

Short-Pulse Operation of Synchrotron Radiation Sources — •Anke-Susanne Müller — Karlsruhe Institute of Technology

Short-pulse operation of synchrotron light source storage rings can be useful for both the production of IR and (coherent) THz-band radiation and high repetition rate pump-probe science in the X-ray regime. Amongst the different approaches to short-pulse generation, in particular the use of dedicated magnet optics for short (ps) electron bunches and the technique of Coherent Harmonic Generation for the production of coherent THz and UV radiation, respectively, will be discussed in this talk.

Invited Talk MI 7.2 Wed 15:30 MOL 213

Progress in White Beam Diffraction Imaging — •Andreas Danilewsky — Kristallographie, Universität Freiburg, Freiburg

Monochromatic X-ray diffraction imaging (topography) has been used for over half a century for the characterization of extended defects such as dislocations, slip bands, stacking faults, etc. in single crystals and devices fabricated thereupon. The advantage of using the synchrotron white beam is a Laue pattern of reflections on X-ray sensitive film, each containing a topograph from the same sample volume. It allows a fast Burgers vector analysis, even in case of high dislocation densities and in high absorbing crystals. The actual development of fast and high resolving indirect digital detector systems supports a tremendous reduction of the exposure time for a single diffraction image. Integration times of less than 0.2 s allow e.g. the real-time metrology of 450 mm Si wafers in less than 4 hours or the in-situ topography at high temperatures to analyse dislocation dynamics in Si or GaAs. A very promising new development is the 3-dimensional diffraction imaging. It results from the 3-dimensional rendering of a high number of section transmission topographs across the sample with the beam collimated to 15 μm and a step size of 15 μm. This new approach allows the measurement of the absolute strain value around defects.

Invited Talk MI 7.3 Wed 16:00 MOL 213

Short pulses @ SOLEIL: Femto-Slicing and Low-Alpha — •Marie Labat — SYnchrotron SOLEIL - Saint-Aubin - FRANCE

In order to produce shorter pulses of synchrotron radiation, two setups have been studied at SOLEIL. Operation in low-alpha mode now enables to deliver few ps pulses to users on several beamlines. And a femto-slicing experiment is presently under commissioning. In the magnetic field of a wiggler, the electron bunch interacts with a Ti:Sa laser of 50 fs-fwhm pulse duration. The energy modulation over this short slice is used to separate it spatially from the core beam in different undulators downstream, allowing the delivery of about 100 fs-fwhm pulses to at least two beamlines. We will report on the commissioning of this femto-slicing experiment and on the operation in low-alpha mode.

Invited Talk MI 7.4 Wed 16:30 MOL 213

Nanomagnets and artificial multiferroics studied with X-ray photoemission electron microscopy — •Frithjof Nolting — Paul Scherrer Institut, Switzerland

Bringing different materials in contact at the nanoscale opens the door to improving or creating new functionalities by tuning the properties of the resulting interfaces. Employing photoemission electron microscopy (PEEM) and X-ray magnetic circular dichroism (XMCD) their magnetic properties can be studied. Using recent results I will explain the technique and its possibilities. One example is the study of the magnetic properties and scaling laws of nanoparticles, were we discovered a size-dependent transition from a single domain state to a non-collinear spin structure in isotropic nanoparticles with sizes ranging from 25 down to 5 nm [1]. A second example will be the demonstration of in situ 90 degree electric field-induced uniform magnetization rotation in single domain submicron ferromagnetic islands grown on a ferroelectric single crystal [2]. Further examples will be about patterned magnetic nanostructures and how the magnetization of ferromagnetic systems can be manipulated by ultrashort laser pulses studied with time resolved measurements [3].

[1]A. Fraile-Rodríguez et al. Phys. Rev. Lett. 104, 127201 (2010).
[2]M. Buzzi et al. Phys Rev. Lett. 111, 027204 (2013).
[3]L. Le Guyader et al. App Phys. Lett. 101, 022410 (2012).

MI 7.5 Wed 17:00 MOL 213

Plans for EEHG and Femtoslicing at DELTA — •Robert Molo, Svenja Hilbrich, Markus Höner, Holger Huck, Maryam Huck, Shaukat Khan, Arne Meyer auf der Heide, Carsten Mai, Helge Rast, Andreas Schick, and Peter Ungelenk — Center for Synchrotron Radiation (DELTA), TU Dortmund University, D-44221 Dortmund, Germany

In order to reach shorter wavelengths, the short-pulse facility based on the Coherent Harmonic Generation (CHG) technique at DELTA, a 1.5-GeV synchrotron light source operated by the TU Dortmund

University, will be upgraded using Echo-Enabled Harmonic Generation (EEHG). Both the CHG and the EEHG scheme employ a laser-induced energy modulation, which additionally can be used to generate ultrashort pulses of incoherent radiation at arbitrary wavelengths by transversely displacing the off-energy electrons (femtoslicing). A new storage ring lattice will be presented that not only offers enough space for an EEHG and femtoslicing setup, but also allows to operate both radiation sources simultaneously.

MI 8: Poster: Microanalysis and Microscopy

Chair: Enrico Langer (TU Dresden), Hartmut S. Leipner (Martin-Luther-Universität Halle-Wittenberg)

Time: Wednesday 17:00–19:30 Location: P4

MI 8.1 Wed 17:00 P4

Development of a μm-positron beam for non-destructive 3D-defect imaging — •Thomas Gigl, Markus Reiner, Christian Piochacz, and Christoph Hugenschmidt — Technische Universität München, Physik-Department E21 and FRM II, 85748 Garching

Doppler broadening spectroscopy with positrons is a well-established non-destructive tool for the investigation of lattice defects in solids. The positron as a nanoprobe is highly sensitive to open volume defects, vacancy-atom complexes and atom clusters of higher positron affinity. The chemical surrounding of the annihilation site can be studied by the coincident detection of the Doppler shifted quanta. For the current project a new high resolution Coincident Doppler Broadening (CDB) spectrometer is under development at the high intensity positron source NEPOMUC (Neutron induced Positron source MUniCh) at the research neutron source FRM II. Therefore, a brightness enhancement system consisting of a Ni(100) re-moderation foil and different magnetic and electrostatic lenses have to be designed and simulated. The aim is to reach a positron beam diameter of below a few μm at the sample position for high resolution experiments. Within this contribution the new design of the spectrometer and simulations to the brightness enhancement system will be presented. Financial support provided for the improvement of the instruments PAES and CDBS (project nos. 05KI0WOB and 05K13WO1) by the BMBF is gratefully acknowledged

MI 8.2 Wed 17:00 P4

Improved algorithm for the determination of the Fermi surface in correlated systems using positrons — •Josef Andreas Weber[1], Hubert Ceeh[1], Liviu Chioncel[3], Christoph Hugenschmidt[1,2], Michael Leitner[1], and Peter Böni[1] — [1]Technische Universität München, Physik Department, Lehrstuhl E21, James-Franck-Straße, D-85748 Garching, Germany — [2]Technische Universität München, Forschungs-Neutronenquelle Heinz Maier-Leibnitz, Lichtenbergstraße 1, D-85748 Garching, Germany — [3]University of Augsburg, Theoretical Physics III, D-86135 Augsburg, Germany

The two-dimensional measurement of the angular correlation of the positron annihilation radiation (2D-ACAR) is a powerful tool to investigate the electronic structure of materials. In order to extract the Fermi surface a reconstruction from the measured projections of the electron momentum density is necessary. We will present an improved algorithm taking into account the full symmetry of the problem and the experimental resolution. It is shown, that this procedure will facilitate the comparison between measured data and ab-initio calculations in correlated electron systems. This circumstance is demonstrated by the reconstruction of the Fermi surfaces of nickel and copper.

MI 8.3 Wed 17:00 P4

Analyse leichter Elemente mittels Kernreaktionsanalyse an der Ionenstrahlmikrosonde — •Christian Freiherr[1], Fabienne Eder[3], Silke Merchel[1], Frans Munnik[2], Christian Neelmeijer[2] und Axel D. Renno[1] — [1]Helmholtz-Institut Freiberg für Ressourcentechnologie (HIF) — [2]Helmholtz-Zentrum Dresden-Rossendorf (HZDR) — [3]TU Wien

Ein etabliertes Verfahren der chemischen Analyse mittels Ionenstrahlen ist die simultane Anwendung verschiedener Methoden wie Rutherford Backscattering Spectrometry (RBS), Particle-Induced X-Ray Emission (PIXE), Nuclear Reaction Analysis (NRA) und Particle-Induced Gamma Emission (PIGE). Am Ionenstrahlzentrum des HZDR haben wir die Möglichkeit, derartige Messungen mit einem fokussierten Ionenmikrostrahl durchzuführen, welcher eine laterale Auflösung von bis zu $3 \times 3\,\mu m^2$ liefert. Zur Zeit liegt der Schwerpunkt unserer Arbeiten auf der quantitativen Analyse von Lithium, Bor und Fluor. Die Messung derart leichter Elemente wird durch die isotopensensitiven Methoden PIGE und NRA ermöglicht. Hierbei werden durch die beschleunigten Projektilionen Kernreaktionen mit den Atomen der Probe induziert und deren Reaktionsprodukte (Photonen bzw. massive Teilchen) detektiert. Die Eignung verschiedener Kernreaktionen wird diskutiert und erste Resultate anhand untersuchter Referenzmaterialien und geologischer Proben vorgestellt. Zudem werden – dank der Zerstörungsfreiheit der Methoden – hochsensible Kunst- und Kulturgutproben untersucht.

MI 8.4 Wed 17:00 P4

Determination of trap and band states in organic field-effect transistors by scanning Kelvin probe microscopy — •Sebastian Hietzschold[1,2], Michael Scherer[2,3], Janusz Schinke[2,3], Robert Lovrincic[2,3], and Wolfgang Kowalsky[2,3] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Germany — [2]InnovationLab, Heidelberg, Germany — [3]Institut für Hochfrequenztechnik, Technische Universität Braunschweig, Germany

We determine the density of states (DOS) including gap states in organic semiconductors by means of scanning Kelvin probe microscopy (SKPM). We apply this energy resolving technique with high spatial resolution to bottom gate organic field-effect transistors (OFETs) using the small molecule organic semiconductor pentacene on either HMDS modified or unmodified silicon dioxide gate dielectric. Biasing the gate electrode leads to a filling and emptying of electronic states in the semiconductor resulting in a shift of the surface potential. Hereby we indirectly gain the density of trap as well as band states. The measurements were performed in both ambient atmosphere and ultra-high vacuum. Additionally we compare the results to transistors made of Poly[bis(4-phenyl)(2,4,6-trimethylphenyl)amine] (PTAA) which is widely used as an air stable solution processable organic p-type semiconductor. The DOS of PTAA exhibits several additional peaks compared to pentacene, probably related to impurity induced energy levels and a higher degree of structural disorder. Finally, we correlate the obtained DOS distributions to the device performances.

MI 8.5 Wed 17:00 P4

Sensitivity in SubSurface-AFM: Tip-Sample Interaction in Heterodyne Force Microscopy — •Gerard J. Verbiest[1], Tjerk H. Oosterkamp[2], and Marcel J. Rost[2] — [1]JARA- FIT and II. Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]Kamerlingh Onnes Laboratory, Leiden University, P.O. Box 9504, 2300 RA Leiden, The Netherlands

A couple of reported Heterodyne Force Microscopy (HFM) measurements demonstrate the unique possibility to nondestructively image 20 nm small nanoparticles buried 500 nm below a surface with an AFM. HFM utilizes two ultrasonic signals of slightly different frequencies that are sent through the sample and the cantilever, respectively. The sound wave through the sample contains subsurface information and access to it is possible, as the nonlinear interaction between the cantilever's tip and the sample generates a low-frequency heterodyne force that can be detected in the cantilever's motion, if one tunes this force below its fundamental resonance frequency. A quantitative analysis of the measurements and the determination of their contrast mechanism is only possible with a detailed understanding of the nonlinear dynamics.

We present an experimental and a numerical study of the cantilever motion in HFM, where the two ultrasonic frequencies and the heterodyne frequency are far from any resonance of the cantilever [1,2]. The results provide information on the sensitivity to subsurface features and deliver a recipe for the experimental settings of the frequencies.

[1] G.J. Verbiest et al., Ultramicroscopy 135, 113 (2013)
[2] G.J. Verbiest et al., Nanotechnology 24, 365701 (2013)

MI 8.6 Wed 17:00 P4

Prototyping of Cobalt MFM tips with high spatial resolution using electron beam induced deposition — •Johannes J.L.

Mulders and Daniela Sudfeld — FEI Electron Optics B. V., Eindhoven, The Netherlands

The fast creation of MFM cantilevers for magnetic force microscopy studies is a challenge for many conventional lithography techniques. Electron beam induced deposition is a direct write patterning technique, using the electron beam of a scanning electron microscope (SEM) to locally dissociate injected precursor molecules adhered to a surface. The details are described elsewhere [1], but in 3 minutes a tip can be made without clean room environment. With FEI EBID technique, MFM tips in the form of Co spike tips with a lateral resolution of 10 nm were produced [2]. In addition, the magnetic spatial resolution for those MFM cantilevers is improved and measurements with those tips indicated a better signal-to-noise performance [2]. The vertical growth is controlled by the dwell time and very accurate on the nano-scale regime due to the 3 dimensional, mask-free patterning. That allows to tailor the shape of the tip to enhance the performance. The life time and stability of tips can be increased by additional carbon coating preventing natural oxidation. [1] Utke I, Moshkalev S, Russell P: Nanofabrication Using Focused Ion and Electron Beams, Chapter 10, Oxford University Press (2012; [2] L. M. Belova et al., Rev. Sci. Instrum. 83, 093711 (2012)

MI 8.7 Wed 17:00 P4

Imaging applications and fabrication process of x-ray waveguides — •Sarah Hoffmann, Henrike Neubauer, Mike Kanbach, Anna-Lena Robisch, and Tim Salditt — Institut für Röntgenphysik, Friedrich-Hund Platz 1, 37077 Göttingen

Nanoscale x-ray sources as provided by x-ray channel waveguides enable a multitude of novel applications such as diffraction, high resolution spectroscopy, microscopy and holography [1,2].We report on imaging experiments and the fabrication process of these hard x-ray waveguides deployed at the synchrotron source DESY, PETRA III/P10. Among other techniques e-beam lithography, reactive ion etching and Silicon wafer bonding are involved within the fabrication of two-dimensional, sub-100 nm sized waveguide channels. Both waveguide geometry and material can be adapted to meet the requirements of a specific experiment, such as the photon energy (7.9-17.5 keV), the desired source size, or the application of a reference beam in a holography setup. As the tunability of the optical properties provided by the waveguides, such as the coherence of the beam, its divergence or the waveguide transmission, depends sensitively on the precise control over the (several) process steps, an iterative process of diagnostics and optimization is essential.

[1] A. Jarre et al., Phys. Rev. Lett. 94, 074801 (2005)
[2] C. Krywka et al., J. Appl. Cryst. 45, 85-92 (2012)
[3] A. Kohlstedt et al., Appl. Phys. A 91, 6-12 (2008)
[4] H. Neubauer et al., in preparation

MI 8.8 Wed 17:00 P4

Diffractive Optics Research at Max Planck Institute for Intelligent Systems in Stuttgart — •Kahraman Keskinbora, Umut Tunca Sanli, Marcel Mayer, Corinne Grévent, and Gisela Schütz — Max Planck Institute for Intelligent Systems, 70569, Stuttgart, Germany

We develop new nano-fabrication methods for advanced focusing optics called Fresnel zone plates (FZP). One of these methods, implies a combination of the atomic layer deposition (ALD) and the focused ion beam (FIB), and allows to fabricate FZPs having outermost zone widths as small as 10 nm with extremely high aspect ratios compared to the FZPs fabricated by e-beam lithography (EBL). Moreover, we have demonstrated that these zone plates can actually work efficiently over a wide energy range from soft to hard X-rays. Our current research covers the improvement and optimization of the material selection of the ALD deposition process and FIB slicing/polishing. In another fabrication method, we utilize the direct writing capabilities of the FIBs for ultra-rapid fabrication of FZPs with features as small as 30 nm. It was possible to resolve features down to 21 nm. The fabrication lasts less than 9 minutes and the resolution is close to those of standard EBL-FZPs, which is remarkable. We are working towards improving resolutions and diffraction efficiencies of IBL-FZPs by pattern design and process optimizations as well as material improvements

MI 8.9 Wed 17:00 P4

Status and upgrades of the MAXYMUS X-ray microscope — •Iuliia Bykova, Markus Weigand, Michael Bechtel, Claudia Stahl, Eberhard Goering, and Gisela Schütz — Max-Plank-Institute for Intelligent Systems, Stuttgart, Germany

MAXYMUS is an Ultra-High Vacuum (UHV) Scanning Transmission X-ray Microscope (STXM) operated by the MPI for Intelligent Systems at a dedicated soft X-ray undulator beamline at the Bessy II synchrotron (Berlin, Germany) with the feasibility of high brightness and selectable polarization measurements. MAXYMUS is a fully UHV compatible and sensitive for surface current measurements at pressures below $5 \cdot 10^{-9}$ mBar. Also, it is custom-built photon counting and synchronization setup that allows efficient time resolved experiments with the resolution of < 100 ps. These characteristics make MAXYMUS one of the world leading devices in magnetic imaging. We will show results which were obtained due to mentioned features as well as additional options like adjustable magnetic field setups, goniometric and cryostat sample holders, enabling sample temperatures of 80 to 500 K. Currently, MAXYMUS is undergoing an extensive upgrade, which includes the introduction of a new control software and interferometer feedback system as well as a fast in-vacuum CCD camera. The capability of energy-sensitive single photon detection at rates up to 1000 fps will allow drastic increase in resolution and throughput by the use of ptychography and soft X-ray fluorescent microscopy.

MI 8.10 Wed 17:00 P4

Study of core-shell nanowires by kinematic scattering theory — •Thilo Krause and Michael Hanke — Paul Drude Institut für Festkörperelektronik, Hausvogteiplatz 5-7, D-10117 Berlin, Germany

We investigate GaAs/InGaAs/GaAs core-shell nanowires with respect to strain and morphology. We vary parameters such as Indium concentration and shell thickness which can also be controlled during the nanowire growth. For different models we perform kinematic scattering simulations based on the finite element method (FEM). From this we are able to analyze the total elastic strain. The kinematic scattering simulations shall be compared to experiments performed at a synchrotron nano-probe beamline with a spot size of about 100 nm in diameter. Such highly focused beams enable X-ray diffraction experiments on single nanowires and small ensembles.

MI 9: Functional Materials - Analysis with EBSD, X-Ray Kossel Diffraction and Related Methods (MI jointly with KR)

Chair: Enrico Langer (TU Dresden)

Time: Thursday 9:30–11:00 Location: MER 02

Invited Talk MI 9.1 Thu 9:30 MER 02

The martensitic transformation in Co-Ni-Al F-SMA — •Jaromír Kopeček[1], Karel Jurek[1], Michal Landa[2], and Oleg Heczko[1] — [1]Institute of Physics ASCR, Praha, Czech Republic — [2]Institute of Thermomechanics ASCR, Praha, Czech Republic

The Co-Ni-Al alloys were in the focus of physicist from the beginning of research in ferromagnetic shape memory alloys, but as the surprisingly higher and higher magnetic field induced strain due to reorientation or transformation in magnetic field were announced in Ni-Mn-Ga system, the more dubious results emerged for the Co-Ni-Al system. It seemed apparent that Co-based shape memory alloys would quickly return into the structural intermetallics, interesting, complicated and useful, but just as another superalloy. Despite the knowledge accumulated in literature, recently researchers in this field were frustrated by curious disagreement between optical observation showing martensite lamellae at room temperature while magnetic measurement indicates that the martensitic transformation is well below zero. The present work compiled the results of various methods, which - we believe - proved that the martensitic transformation temperature in $Co_{38}Ni_{33}Al_{29}$ is around -70 °C, whereas all higher temperature features are examples of stress induced transformation. Using various microscopies including EBSD together with RUS, magnetic measurements and mechanical testing we were able to explain the evolution of the structure. In comparison with Ni-Mn-Ga systems there are marked differences in transformation path which ultimately may explain why we cannot expect the magnetic shape phenomena in Co-Ni-Al alloys.

MI 9.2 Thu 10:00 MER 02

Charakterisierung flächenhafter Inhomogenitäten in der ferromagnetischen Formgedächtnislegierung $Co_{38}Ni_{33}Al_{29}$ mittels Kossel- und Pseudo-Kossel-Technik — Enrico Langer[1,2], Siegfried Däbritz[1], •Leonid P. Potapov[1], Katerina Kratka[1] und Jaromír Kopeček[3] — [1]Technische Universität Dresden, Institut für Festkörperphysik, 01062 Dresden, Germany — [2]Technische Universität Dresden, Institut für Halbleiter- und Mikrosystemtechnik, 01062 Dresden, Germany — [3]Academy of Sciences of the Czech Republic, Insitute of Physics, 18222 Prague, Czech Republic

Die Legierung $Co_{38}Ni_{33}Al_{29}$ weist unter den ferromagnetischen Formgedächtnissystemen besonders gute werkstoffphysikalische Eigenschaften auf, wie beispielsweise gute Korrosionsbeständigkeit und ausgeprägte Duktilität. Beobachtete flächenhafte Inhomogenitäten zeichnen sich im Rückstreuelektronenkontrast dunkel gegenüber der Probenmatrix aus und befinden sich innerhalb der B2-β-Phase des Austenit-Kristalls der ferromagnetischen Legierung. Insbesondere heben sie sich als dunkle Ränder in der β-Phase nahe der Phasengrenze und als dunkle periodische Strukturen hervor.

Die Kossel-Technik liefert zur Charakterisierung dieser Gebiete aufschlussreiche Ergebnisse bezüglich der Kristallqualität. Es zeigt sich erstens, dass die genannten Randstrukturen eine exakte Ausrichtung nach der Kurdjumov-Sachs-Orientierungsrelation bestätigen und zweitens, dass die beobachtete Reflexüberlagerung in den A1- bzw. B2-Phasen die Kossel-Reflexe (111) und (002) beziehungsweise (110) und (011) betreffen. Außerdem besitzt die periodisch dunkle Struktur innerhalb der β-Phase eine komplizierte rechteckige Anordnung von Punkten, verbunden durch sehr feine Linien. Diese periodische Struktur richtet sich offensichtlich entlang der Kristallwachstumsrichtung [100] aus. Pseudo-Kossel-Aufnahmen bestätigen ebenfalls erfolgreich eine Kristallqualitätsverbesserung in den dunklen Gebieten, was sich durch eine lokale Verschärfung einzelner Interferenzreflexe vom Typ (110) äußerte.

MI 9.3 Thu 10:15 MER 02

Strain inhomogeneities in epitaxial $BaFe_2As_2$ thin films measured by cross correlation electron backscatter diffraction — •Paul Chekhonin[1], Jan Engelmann[2], Bernhard Holzapfel[2], Carl-Georg Oertel[1], and Werner Skrotzki[1] — [1]Institut für Strukturphysik, Technische Universität Dresden — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden

Epitaxial thin films of strained $BaFe_2As_2$ have been produced by pulsed laser deposition on a spinel substrate with an iron buffer layer. Using the cross correlation electron backscatter diffraction technique in a scanning electron microscope, relative measurements of very small strains and disorientations are possible. From electron backscatter diffraction pattern obtained on the $BaFe_2As_2$ layer partially strain relaxed areas were measured. Additionally, strain inhomogeneities and disorientations on length scales of few 100 nm and smaller have been detected.

MI 9.4 Thu 10:30 MER 02

Simulation of phase propagation delay for modulated EBIC in thin Silicon samples — •Markus Holla, Markus Ratzke, Winfried Seifert, and Martin Kittler — Joint Lab IHP/BTU, BTU Cottbus, Konrad-Wachsmann-Allee 1, 03046 Cottbus, Germany

Calculations of locally induced currents by a modulated electron beam are presented for thin Silicon samples with Schottky contacts. The theoretic electron beam current (EBIC) amplitudes and phase shifts are analyzed to estimate the influence of semiconductor parameters (such as surface recombination velocity, diffusion length and diffusion coefficient). The parameter identification limits for the method are discussed. Among other results it was found, that the phase shift correlates with the diffusion coefficient. The surface layer interaction and the resulting effective diffusion length behavior are presented, too.

MI 9.5 Thu 10:45 MER 02

Characterization of 0-3 high permittivity composite capacitors for energy storage — •Jens Glenneberg, Gerald Wagner, Thomas Grossmann, Stefan Ebbinghaus, Martin Diestelhorst, Sebastian Lemm, Horst Beige, and Hartmut Leipner — Martin-Luther-Universität Halle-Wittenberg

Energy storage is more than ever an important topic, while thin film capacitors with high energy densities seem to be a promising solution. Their advantages over accumulators are for example quick charging and discharging times, long lifetimes and low manufacturing costs.

Due to its ferroelectric properties and extremely high permittivity, $CaCu_3Ti_4O_{12}$ (CCTO) is well suited for the use in short term energy storage. Since pure CCTO exhibits comparatively low breakdown field strength, the device efficiency is limited. To increase the energy densities, CCTO nanoparticles can be embedded in specific inorganic matrices. The size and distribution of the nanoparticles determine the electric properties of the capacitor dielectrics to a very large extent.

To investigate the microstructure, the nanoparticles and the surrounding matrix are imaged by environmental scanning electron microscopy (ESEM) in both secondary electron contrast (SE) and backscattered electron contrast (BSE) as well as by transmission electron microscopy (TEM). To acquire compositional information, additional energy-dispersive X-ray spectroscopy (EDS) has been carried out. With the help of these investigations an assessment to the chemical composition and the microstructure is allowed, which can be seen in context to the resulting electrical properties.

MI 10: Crystallography in Nanoscience (KR jointly with MI)

Time: Thursday 11:00–11:45 Location: CHE 184

MI 10.1 Thu 11:00 CHE 184

Structure and dynamics of functional guest complexes in porous matrices — •Dominik Schaniel[1], Kuan-Ying Hsieh[1], El-Eulmi Bendeif[1], Axel Gansmuller[1], Sebastien Pillet[1], and Theo Woike[2] — [1]Université de Lorraine, CRM2, UMR 7036, Vandoeuvre-les-Nancy — [2]Institut für Strukturphysik, TU Dresden

The inclusion of functional molecules in nanostructured matrices is a very active field of research due to the potential applications of such hybrid materials, e.g. in optics, catalysis, or even medicine [1-4]. As a key to the understanding of the properties the structure of the host-guest system must be known. We have synthesised such nanohybrids by encapsulation of photoswitchable complexes ($Na_2[(Fe(CN)_5NO]2H_2O$, SNP) into porous silica matrices with different pore sizes from 1 nm to 20 nm. The structural study has been performed using total scattering methods coupled to pair distribution function analysis (PDF) and nuclear magnetic resonance (NMR). The PDF analysis allows for the determination of the structural arrangement of the isolated SNP complexes (cation- anion) as well as the size of the embedded cluster/nanoparticle. NMR reveals a dynamical behaviour of the guest complexes which depends on the hydration level of the matrix.

[1] Sanchez et al., Adv. Mater. 2003, 15, 1669 ; Vinu et al., J. Nanosci. Nanotec. 2005, 5, 347. [2] Deniz et al., Chem. Eur. J. 2012, 18, 15782. [3] Blecher et al., Nanomedicine : Nanotechnology, Biology, and Medicine 2012, 8, 1364. [4] T.-W. Sung, Y.-L. Lo, Sensors and Actuators B : Chemical 2012, 173, 406.

MI 10.2 Thu 11:15 CHE 184

Crystallization behaviors of n-octadecanol on the surface of silica nanosphere — •Yunlan Su[1,2], Xia Gao[1], Dujin Wang[1], and Patrick Huber[2] — [1]Key Laboratory of Engineering Plastics, Institute of Chemistry, Chinese Academy of Sciences, Beijing, China — [2]Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany

Geometrical confinement of materials on the nm-scale is known to have an impact on many physical properties. For example, phase transitions can be entirely suppressed or significantly altered in comparison to their bulk counterparts and the molecular dynamics can be affected markedly, especially in the vicinity of glass transitions. In the work, we designed n-octadecanol/SiO2 nanosphere (d = 90 nm) composites and studied the crystallization behaviors of C18H37OH in nanosized space formed by SiO2 nanospheres by DSC and variable-temperature X-ray diffraction (VT-XRD). The transition temperatures for confined C18H37OH are lower than for bulk C18H37OH; In addition, under confinement, the low temperature ordered phase has changed, probably due to the suppression of mobility of molecular chain. While bulk C18H37OH exhibits a crystalline phase of γ form, geometrical confinement favors a mixture of γ and β phases. Geometrical confinement favors a phase closely related to the β form, in which the crystallites with an orthorhombic subcell and chain axes are parallel to the bilayer normal are formed. A reason for this might be the confinement effect, into which the crystallites have to fit, favoring the formation of the geometrically more simple and less bulky form.

MI 10.3 Thu 11:30 CHE 184

Mapping the velocity field around a micro-oscillator in water — •Spas Nedev[1], Sol Carretero-Palacios[1], Silke R. Kirchner[1], Frank Jäckel[1,2], and Jochen Feldmann[1] — [1]Photonics and Optoelectronics Group, Physics Department and Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München, Amalienstr. 54, 80799 Munich, Germany — [2]Department of Physics and Stephenson Institute for Renewable Energy, University of Liverpool, Chadwick Building, Peach Street, Liverpool, L69 7ZF, United Kingdom

Optical trapping in combination with microfluidics provides novel analytical and sensing capabilities. Here we show an experimental and theoretical approach to detect and map the velocity field around a micro-oscillator in water. Fluidic vibrations created by a micro-source, an optically trapped silica particle set to oscillate in a dipole-type mode, lead to displacement of another twin silica particle independently trapped in its vicinity acting as a detector. Fourier analysis of the motion of the detecting particle at different points in space and time provides the velocity map around the oscillating microsphere. The combination of measured velocity field and microfluidic theoretical models reveals that the measured fields are dominated by microfluidic contributions, with a significant acoustic contribution. The concept introduced here allows for the study of the fluidic and acoustic near fields close to micro-source in water. Furthermore it serves a basis for nano-positioning system for location and recognition of moving sources that may be applied to artificial micro-objects and living organisms.

MI 11: Crystallography in Materials Science (KR jointly with DF, MI)

Time: Thursday 15:00–17:30 Location: CHE 184

Invited Talk MI 11.1 Thu 15:00 CHE 184

Crystals: Structure, Properties and Heart of Energy Conversion Devices — •Tilmann Leisegang[1], Juliane Hanzig[2], Erik Mehner[2], Matthias Zschornak[2], Falk Meutzner[2], Tina Nestler[2], Bianca Störr[2], Charaf Cherkouk[2], Ulrike Wunderwald[1], and Dirk C. Meyer[2] — [1]Fraunhofer-THM, Am-St.-Niclas-Schacht 13, 09599 Freiberg — [2]TU Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Str. 23, 09596 Freiberg

Crystalline materials are wide spread in our today's life. More than 98 % of the solid fraction of the earth comprises crystalline matter, most of which are oxides. Single-crystals in particular are the basis for many applications - lasers, LEDs, sensors, etc. - and play an important role in fundamental research for instance in superconductivity or magnetic properties. The discipline that elucidates the impact of the crystal structure on the physical properties of particularly crystalline materials - crystallography - is of specific importance for the design of new materials. X-ray and other diffraction methods are of great relevance for the investigation of crystal structures and their peculiarities. Moreover, crystallography can be utilized to establish new concepts and thus may contribute solving today's challenges in science and technology. In this context, the work presented highlights several examples. First, it is demonstrated how composition variations can be used to change the three dimensional crystal structure - including commensurate or incommensurate modulated phases - in order to tune the materials properties. Second, applications of crystals for energy conversion devices are presented.

MI 11.2 Thu 15:30 CHE 184

Clusters in intermetallic compounds: fullerenes and more — •Julia Dshemuchadse and Walter Steurer — Laboratory of Crystallography, Department of Materials, ETH Zurich, Switzerland

The study of the structure of metals has kept crystallographers busy for the past century: starting with the simplest of structures – sphere packings, such as found in aluminium or copper – up to some of the most complex inorganic structures known to date with more than 20 000 atoms per unit cell [1]. But knowing all the atomic positions does not yet provide us with a deeper understanding of the design of the structure.

Different cluster interpretations of the atomic arrangement in an intermetallic can provide us with recurring motifs in the form of atomic environments, *i.e.* coordination polyhedra, or larger, endohedral clusters, such as dual Frank-Kasper polyhedra and fullerene-like shells (*e.g.*, [2]). These cluster descriptions illustrate common features in structures either within the same intermetallic system or of related structures with entirely different constituents. However, they do not necessarily represent chemical entities and their meaningfulness is usually derived from their repeated occurrence in diverse compounds.

We will present possible ways of structure description for complex intermetallic phases and clues toward their significance.

[1] T. Weber, J. Dshemuchadse, M. Kobas, M. Conrad, B. Harbrecht and W. Steurer, *Acta Cryst. B* 65, 308–317 (2009).

[2] J. Dshemuchadse, S. Bigler, A. Simonov, T. Weber, W. Steurer, *Acta Cryst. B* 69, 238–248 (2013).

MI 11.3 Thu 15:45 CHE 184

Theoretical investigation of the high pressure structure of CaTe — •Oliver Potzel and Gerhard Taubmann — Institute of Theoretical Chemistry, University of Ulm, D-89069 Ulm, Germany

The majority of the alkaline halides and the alkaline earth chalcogenides undergoes a structural phase transition from the B1 (rock-salt) structure to the B2 (CsCl) structure at elevated pressures [1].

The x-ray diffraction data of CaTe at high pressures (320 - 400 kbar) fit to a simple cubic indexing (B2) except for two reflections near the (110) peak [2]. This indicates the possible existence of an intermediate structure within the transition from the B1 to the B2 structure.

We are currently using the evolutionary algorithms of the USPEX code [3] with the periodic DFT code VASP [4] in order to predict the structure of CaTe at a pressure of 350 kbar.

Preliminary DFT studies without genetic algorithms pointed to an AgO structure. In these calculations, all known (binary) AB structures were taken into account.

The results are to be verified by the comparison of the calculated data to the experimental diffraction data.

[1] O. Potzel, G. Taubmann, J. Solid State Chem. 184, 1079 (2011)
[2] H.G. Zimmer, H. Winzen, K. Syassen, PRB 32, 4066 (1985)
[3] A.R. Oganov , C.W. Glass, J. Chem. Phys. 124, 244704 (2006)
[4] G. Kresse, J. Furthmüller, PRB 54, 11169 (1996)

MI 11.4 Thu 16:00 CHE 184

In-situ ion beam irradiation: X-ray scattering & diffraction experiments — Olga Roshchupkina, Carsten Baehtz, Stefan Facsko, Lothar Bischoff, Matthias Posselt, and •Joerg Grenzer — Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden

Ion beam techniques are widely used in semiconductor industry e.g. for introducing dopant atoms into materials. Ion implantation is characterized by fast dynamic processes associated with the evolution of collision cascades resulting in formation of defects such as vacancies, interstitials, etc. As a consequence, typically a strained layer that expands in the direction normal to the substrate surface is formed. This is due to the fact that the bulk material prevents any lateral macroscopic expansion and as a result the thin irradiated layer is subjected to an in-plane biaxial compressive stress. Ion irradiation is a very fast process and it is almost impossible to monitor it in-situ with the present x-ray sources. However, the accumulation of damage and the diffusion of defects are much slower processes and can be studied in-situ by X-rays. An in-situ ion beam implantation experiment was set up at ROBL/MRH at ESRF. Samples were irradiated using 20 keV He^+ ions at room temperature. Reciprocal space maps to investigate the evolution of the strain depending on the accumulation of defects, as well as the conversion of the strained layer into a completely (X-ray) amorphous layer on single crystal Si and Al_2O_3 substrates were measured and discussed.

Coffee break

MI 11.5 Thu 16:30 CHE 184

Focused Ion Beam implantation of Erbium into Y2SiO5 crystals — •Nadezhda Kukharchyk[1], Jasper Rödiger[2], Arne Ludwig[1], Alexey Ustinov[3], Pavel Bushev[4], and Andreas D. Wieck[1] — [1]Ruhr University Bochum, Bochum — [2]RUBION, Bochum — [3]Karlsruhe University, Karlsruhe — [4]University of Saarland, Saarbrücken

In the context of research on quantum computation and information, different systems have been developed and investigated recently. Particular interest is focused on the systems based on the rare earth (RE) elements, which feature semi-shielded 4f-electrons from external crystal fields and therefore possess long optical and microwave coherence time. Among all the REs, exclusively erbium has the transition which falls into Telecom C-Band at 1540 nm. In the present work, we perform Focused Ion Beam (FIB) implantation of Erbium ions into Y2SiO5 substrates. The FIB allows us to have a high control over the implanted pattern and area, as well as the depth and even the choice of the isotopes - which gives high flexibility in the system preparation. Luminescence of the implanted crystals appears to be an effective way to characterize the system. The measurements were performed in the confocal regime with an excitation at 488 nm and detection in the range of 450 nm to 900 nm at room temperature. A marked intensity-to-fluence dependence is observed and compared to the spectra from the grown doped crystals. Additionally the influence of defects and annealing was studied.

MI 11.6 Thu 16:45 CHE 184

White beam synchrotron x-ray topography of sapphire single crystals — •Atefeh Jafari[1,2], Angelica Cecilia[3], Jürgen Härtwig[4], Andreas Danilewsky[5], Dimitrios Bessas[4], Viktor Asadchikov[6], Boris Roschin[6], Denis Zolotov[6], Alexander Deryabin[6], Ilya Sergeev[7], Svetoslav Stankov[3], Tilo Baumbach[3], Pavel Alexeev[1,7], Hans-Christian Wille[7], and Raphaël Hermann[1,2] — [1]Jülich Centre for Neutron Science JCNS and Peter Grünberg Institute PGI, JARA-FIT, Forschungszentrum Jülich, Germany — [2]Faculté des Sciences, Université de Liège, Liège, Belgium — [3]Institute for Photon Science and Synchrotron Radiation, KIT, Germany — [4]European Synchrotron Radiation Facility, Grenoble, France — [5]Crystallographic institute, University of Freiburg,Germany — [6]Shubnikov Institute of Crystallography, RAS, Moscow, Russia — [7]Deutsches Elektronen-Synchrotron, Hamburg, Germany

Sapphire single crystals grown by different techniques have been assessed with white beam and meV-resolution synchrotron x-ray topography at ANKA, KIT and PETRA III, DESY, and ESRF, respectively. Excellent crystal quality is required for the use in backscattering x-ray monochromators for nuclear resonance scattering with resonance energies above 30 keV. X-ray topography reveals defects and dislocations and hints at their origin. Crystals grown by the Kyropoulos method show the lowest dislocation density. Support of the Helmholtz-Russia joint research group HRJRG-402, ANKA, PETRA III and ESRF is acknowledged.

MI 11.7 Thu 17:00 CHE 184

Improving Nanomagnetometry Based on Nitrogen-Vacancy Centers by Coupling to Superparamagnetic Iron Oxide Nanoparticles — •Nikola Sadzak, Janik Wolters, Andreas W. Schell, Sten Wenzel, and Oliver Benson — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, Berlin, Germany

The single negatively charged nitrogen-vacancy (NV) defect center in diamond is known to be a stable solid-state single photon source [1], with an electronic spin showing long coherence times even at room temperature. Furthermore, the optical readout of the spin state and its microwave-assisted manipulation allow this defect to be used either as a qubit register [2] or as a magnetic field sensor [3]. Here, we perform the coupling of individual NV centers in nanodiamond with single-domain superparamagnetic iron oxide nanoparticles. By showing huge magnetic susceptibilities and no hysteresis, the latter can be used as local microwave amplifiers, allowing the achievement of faster Rabi oscillations between the NV center electronic spin sublevels. Moreover, we investigate the effects on the NV- electronic spin dynamics and coherence times and discuss some applications in NV-based nanomagnetometry.

[1] I. Aharonovich et al., Rep. Prog. Phys. 74, 076501 (2011).
[2] L. Robledo et al., Nature 477, 574-578 (2011).
[3] J. R. Maze et al., Nature 455, 644-648 (2008).

MI 11.8 Thu 17:15 CHE 184

Selective preparation of single-crystalline alpha- & beta-phase perylene platelets — •André Pick and Gregor Witte — Molekulare Festkörperphysik, Philipps-Universität Marburg, 35032 Marburg

Though polarization resolved optical absorption spectroscopy in transmission geometry is a simple method to characterize optoelectronic properties of pi-conjugated molecular crystals their large absorption requires rather thin crystals. Moreover such studies are complicated by the presence of polymorphism and structural defects like twinning. For the case of the polycyclic aromatic hydrocarbon perylene two crystalline phases (alpha and beta) are known which comprise different molecules per unit cell. Both crystalline phases exhibit also characteristic differences in the habitus of single crystals which allows their differentiation. Here, we present a method to selectively prepare thin platelets of both polymorphisms, which are suitable for optical studies of single crystals. In order to get full morphological information, the crystallites were characterized by means of optical microscopy, X-ray diffraction and atomic force microscopy.