Crystallography Division
Fachgruppe Kristallographie (KR)

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Overview of Invited Talks and Sessions

(Lecture rooms: CHE 184, and HSZ 02; Posters: P4)

Invited Talks

KR 13.1	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

Plenary Talk related to Division KR

PV II	Mon	14:00–14:45	HSZ 01	**Diffraction before destruction: Imaging proteins with X-ray free-electron laser pulses** — •Henry Chapman

Invited talks of the joint symposium Crystallography in Materials Science (KR, DF, MA, MI)

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

Sessions

KR 1.1–1.1	Mon	9:30–10:15	GER 37	**Invited Talk - Martin Fally (DF jointly with CPP, TT, KR)**
KR 2.1–2.1	Mon	14:00–14:45	HSZ 01	**Plenary Talk - Henry Chapman**
KR 3.1–3.5	Mon	15:00–17:45	HSZ 02	**Symposium Crystallography in Materials Science**
KR 4.1–4.12	Tue	9:30–12:45	BEY 118	**Multiferroics I (MA jointly with DF, DS, KR, TT)**
KR 5.1–5.13	Wed	9:30–13:00	HSZ 04	**Multiferroics II (MA jointly with DF, DS, KR, TT)**
KR 6.1–6.1	Wed	10:30–11:15	GER 37	**Invited Talk - Stefan Förster (DF jointly with O, DS, KR, MM)**
KR 7.1–7.1	Wed	15:00–15:45	GER 37	**Invited Talk - Heidemarie Schmidt (DF jointly with MA, HL, DS, KR)**
KR 8.1–8.5	Wed	17:00–19:30	P4	**Poster Crystallography**
KR 9.1–9.3	Thu	10:15–11:00	CHE 184	**Recent Developments in X-ray Diffraction**
KR 10.1–10.3	Thu	11:00–11:45	CHE 184	**Crystallography in Nanoscience (KR jointly with MI)**
KR 11.1–11.2	Thu	12:00–12:40	GER 37	**Nano- and microstructured dielectrics (DF jointly with KR)**

KR 12.1–12.5	Thu	9:30–11:00	MER 02	**Functional Materials - Analysis with EBSD, X-Ray Kossel Diffraction and Related Methods (MI jointly with KR)**
KR 13.1–13.8	Thu	15:00–17:30	CHE 184	**Crystallography in Materials Science (KR jointly with DF, MI)**
KR 14	Thu	17:45–18:30	CHE 184	**Mitgliederversammlung FG Kristallographie**

Annual General Meeting of the Crystallography Division

Thursday 17:45–18:30 CHE 184
The future prospects of the Crystallography Division will be discussed. All members are cordially invited.

KR 1: Invited Talk - Martin Fally (DF jointly with CPP, TT, KR)

Time: Monday 9:30–10:15 Location: GER 37

Invited Talk KR 1.1 Mon 9:30 GER 37

Optics with neutrons using holographic gratings — •Martin Fally[1], Jürgen Klepp[1], Christian Pruner[2], and Yasuo Tomita[3] — [1]Faculty of Physics, Uni Wien, Austria — [2]Department of Materials Science and Physics, Uni Salzburg, Austria — [3]University of Electro-Communications, Tokyo, Japan

All neutron-optical phenomena are governed by the neutron-optical potential or, equivalently, the neutron refractive-index. Thus, an important task in the design of neutron-optical elements is to efficiently pattern the neutron refractive-index of materials. For this purpose we use light-sensitive materials and employ holographic techniques to produce diffraction gratings for neutrons.

After an introduction to the basics of neutron optics and the challenges as compared to light optics I will discuss our recent experiments, where we successfully demonstrated the power of this approach. Two- and three-port beam-splitters as well as free-standing film mirrors for cold and very-cold neutrons were set up by exploiting the Pendellösung interference effect. Another intriguing possibility is offered by holographic gratings containing superparamagnetic nanoparticles to produce business card-size neutron polarizers working in comparably low external magnetic induction. Such devices are being developed at present. Finally, I will give an outlook on novel neutron-scattering instrumentation and techniques which are expected from those advancements.

In collaboration with: I. Drevensek-Olenik, S. Gyergyek, J. Kohlbrecher, P. Geltenbort, R. A. Rupp

KR 2: Plenary Talk - Henry Chapman

Time: Monday 14:00–14:45 Location: HSZ 01

Plenary Talk KR 2.1 Mon 14:00 HSZ 01

Diffraction before destruction: Imaging proteins with X-ray free-electron laser pulses — •Henry Chapman — Center for Free-Electron Laser Science, DESY, Hamburg, 22607 Germany — Department of Physics, Hamburg University, 22761 Germany — Center for Ultrafast Imaging, Hamburg, 22761 Germany

The ultrafast pulses from X-ray free-electron lasers have opened up a new method for structure determination of macromolecules. These pulses are of high enough intensity and of sufficiently short duration that individual single-shot diffraction patterns can be obtained from a sample before significant radiation damage occurs. This "diffraction before destruction" method may enable the determination of structures of proteins that cannot be grown into large enough crystals or are too radiation sensitive for high-resolution crystallography. Ultrafast pump-probe studies of photoinduced dynamics in proteins or other materials can also be studied. We have carried out experiments in coherent diffraction from protein nanocrystals, including membrane bound proteins, at the Linac Coherent Light Source (LCLS) at SLAC. The crystals are delivered to the pulsed X-ray beam in a continuously flowing liquid jet, allowing the collection of millions of diffraction patterns that are merged. The method has begun to yield new structures and has the potential to increase the rate at which structures can be solved. We aim to be able to obtain structures from the smallest possible crystals of only a single unit cell, i.e. single molecules. A dedicated instrument for serial nanocrystallography will be deployed at the European XFEL in Hamburg.

KR 3: Symposium Crystallography in Materials Science

Time: Monday 15:00–17:45 Location: HSZ 02

Invited Talk KR 3.1 Mon 15:00 HSZ 02

Complexity on Compression: The Crystallography of High-Density Matter — •Malcolm McMahon — School of Physics and Astronomy, The University of Edinburgh, Edinburgh, UK.

The crystal structure of iron was determined at *normal* conditions as long ago as 1917. But what is the structure of iron within *Super-Earth* exoplanets where core conditions approach 10 million atmospheres (1 TPa) and 10,000 K, and where carbon exists as either diamond, or as an exotic metallic form.

Until the early 1990s, the consensus was that at high pressures, all materials would become metallic, and assume high-symmetry, close-packed crystal structures. But the advent of modern crystallographic methods on synchrotron sources in the early 1990s revealed completely different behavior: even the simplest materials underwent phase transition to complex, frequently incommensurate, forms, while metals became semiconductors or insulators. This complexity is thought to arise from the constraints placed on the electronic wave functions due to the Pauli exclusion principle, the need to orthogonalise the wave functions of both core and valence electrons, and the reduction in the available interstitial space at high compression

In this talk I will present results from recent diffraction studies of elemental metallic systems showing some of the extreme complexity observed at high pressures. I will also look at the new opportunities in extreme conditions crystallography offered by x-ray lasers such as the LCLS in the Stanford, and XFEL in Hamburg.

Invited Talk KR 3.2 Mon 15:30 HSZ 02

X-Ray Microscopy with Coherent Radiation: Beyond the Spatial Resolution of Conventional X-Ray Microscopy — •Christian G. Schroer — Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden, Germany

Hard x-ray microscopy has greatly benefited from the high brilliance of modern synchrotron radiation sources and x-ray free-electron lasers (XFELs). Today, the spatial resolution of conventional x-ray microscopes is limited by the x-ray optics to a few tens of nanometers. Scanning coherent diffraction microscopy, also known as ptychography, can overcome this limitation. In ptychography, the sample is scanned through a confined coherent beam, recording at each location of the scan a far-field diffraction pattern. From these data, the complex transmission function (projected complex refractive index) of the sample and the illuminating complex wave field can be reconstructed with a spatial resolution that clearly exceeds the lateral size of the illuminating beam. The spatial resolution in a ptychogram is shown to depend on the shape (structure factor) of a feature and can vary for different features in the object. In addition, the resolution and contrast depend on the coherent fluence on the sample. For an optimal ptychographic x-ray microscope, this implies a source with highest possible brilliance and an x-ray optic with a large numerical aperture to generate the optimal probe beam. Ptychography closes the gap between real space imaging and reciprocal space structure determination and merges these two fields.

[1] A. Schropp, et al., Appl. Phys. Lett. **100**, 253112 (2012).

Invited Talk KR 3.3 Mon 16:00 HSZ 02

Modulated martensite: A scale bridging Lego game for crystallographers and physicists — •Sebastian Fähler — IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — Technische Universität Dresden, Department of Physics, Institute for Solid State Physics, 01062 Dresden, Germany — Technische Universität Chemnitz, Faculty of Natural Sciences, Institute of Physics, D-09107 Chemnitz, Germany

Among various materials exhibiting reversible phase transformations structures with low crystal symmetry, so-called modulated phases, exhibit the best ferroelectric, magnetocaloric or magnetic shape memory properties. Here it is describe how modulated martensite can be

built in a kind of Lego game from simple tetragonal building blocks. It's complex crystallographic (micro-) structure is determined by the boundary conditions during the nucleation process. Though this building principle can be describe in terms of continuum mechanics, it is consistent with first principle calculations. Supported by SPP 1239 and SPP 1599.

15 min break

Invited Talk KR 3.4 Mon 16:45 HSZ 02

Switching of magnetic domains reveals evidence for spatially inhomogeneous superconductivity — •Michel Kenzelmann — Paul Scherrer Institut

The interplay of magnetic and charge fluctuations can lead to novel quantum phases with exceptional electronic properties. Magnetic order in such quantum phases can fundamentally affect the underlying symmetry and generate new physical properties. Importantly, it has been predicted that spin-density wave (SDW) order in a singlet d-wave superconductor is coupled to triplet superconductivity. We performed neutron diffraction studies of the Q-phase SDW [1] in $CeCoIn_5$, and we make two important observations [2]. We observe a complete and extremely sharp SDW domain switching that is unexplained by current microscopic theories for $CeCoIn_5$. Using representational theory, we interpret our experimental results as evidence for the presence of p-wave superconductivity that coexists with d-wave superconductivity and SDW order. The triplet component is of p-wave symmetry, similar to that found in the A-phase of superfluid ^{3}He, and is modulated as a Cooper pair density wave. Our findings identify the Q-phase as a unique quantum phase where d-wave and modulated p-wave superconductivity are coupled to SDW order, and which emerges in a magneto-superconducting quantum critical point [2].

[1] M. Kenzelmann et al, Science 321, 1652 (2008). [2] S. Gerber et al, submitted to Nature Physics (2013).

Invited Talk KR 3.5 Mon 17:15 HSZ 02

The key role of magnetic neutron diffraction in materials science — •Laurent C. Chapon — Institut Laue-Langevin, Grenoble, France

Since the 1950s, neutron scattering, and more specifically diffraction, has been a tool of choice for studying magnetism at the atomic scale. From the very first experimental proof of antiferromagnetism, a phenomenon predicted by Louis Néel, to unveiling how complex multiferroic materials work, the technique has always offered information of crucial importance to build the physical models that are required to explain macroscopic properties of materials. I will review briefly the historical development of magnetic neutron scattering and present key neutron diffraction experiments in recent areas of interest for condensed matter physicists, in particular highlighting the use of the technique for multiferroics and frustrated magnetic systems.

KR 4: Multiferroics I (MA jointly with DF, DS, KR, TT)

Time: Tuesday 9:30–12:45 Location: BEY 118

KR 4.1 Tue 9:30 BEY 118

***Ab initio* study of electronic transport in the Co/PZT-based tunnel junctions** — •Vladislav Borisov[1], Sergey Ostanin[1], Igor Maznichenko[2], Arthur Ernst[1], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

Magnetoelectric coupling at the multiferroic interfaces FM/FE (FM=Co,Fe, FE=$PbTiO_3$,PZT) was studied from first principles. The magnetic interfacial effect, which is controlled by the FE polarization, originates from the charge transfer and d-orbital redistribution of Co/Fe and Ti mediated by the p-states of interfacial oxygens. In PZT, the presence of Zr dopants may locally enhance the effect. We analysed also the spin polarization of tunneling electrons in Co/PTO/Co and Fe/PTO/Co junctions, in which the calculated four-state conductance can account for the ferroelectrically switchable TMR signal observed recently in LSMO/PZT/Co [1].

[1] D. Pantel *et al.*, *NATURE MATERIALS* **11**, 289 (2012).

KR 4.2 Tue 9:45 BEY 118

Tunneling transport and memristive effects in PbTiO3- based multiferroic tunnel junctions — •Andy Quindeau, Marin Alexe, and Dietrich Hesse — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

A gradually tunable resistance effect based on the tunnel electroresistance (TER) of multiferroic tunnel junctions is investigated. The ferroelectric tunnel barrier comprises, a PbTiO3 layer of a few nm thickness, is embedded between two different ferromagnetic layers, viz. La0.7Sr0.3MnO3 and cobalt. In this capacitor geometry an electric bias, applied perpendicularly to the films, results in a direct tunneling current flowing between the two electrodes. The tunnel resistance is dependent on the polarization of the ferroelectric, which is switchable via relatively high voltage pulses. Due to the variation of the pulse parameters a variety of non-volatile resistance states can easily be achieved. These gradually tunable resistance states, characteristic for a memristor device, can be explained by a ferroelectric domain distribution inside the ferroelectric film: Domains with different polarities can coexist inside one capacitor after partial polarization switching and act as parallel connected tunnel barriers with different tunnel resistances. Temperature dependent measurements show the influence of different electron transport mechanisms, which will be discussed. The impact of the memristive states on the tunnel magnetoresistance (TMR) can be shown.

KR 4.3 Tue 10:00 BEY 118

Lattice and polarizability mediated spin activity in EuTiO3 — •Annette Bussmann-Holder[1], Kevin Caslin[1,2], Patrick Reuvenkamp[1], Zurab Guguchia[3], Hugo Keller[3], Reinhard Kremer[1], and Jürgen Köhler[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstr.1, D-70569 Stuttgart, Germany — [2]Brock University, 500 Glenridge Ave., St. Catharines L2S-3A1, Ontario, Canada — [3]Physik-Institut der Universität Zürich, Winterthurerstr. 190, CH-8057 Zürich, Switzerland

EuTiO3 is shown to exhibit novel strong spin-charge-lattice coupling deep in the paramagnetic phase. Its existence is evidenced by an, until now, unknown response of the paramagnetic susceptibility at temperatures exceeding the structural phase transition temperature TS=282K. The extra features in the susceptibility follow the rotational soft zone boundary mode temperature dependence above and below TS. In addition, novel magnetostriction experiments and dielectric constant measurements have been performed which both reveal giant anomalies related to the antiferromagnetic phase transition at TN=5.7K and the structural phase transition at TS. The theoretical modeling consistently reproduces these anomalies and provides evidence that EuTiO3 has considerable analogies to SrTiO3 but also substantial differences stemming from the Eu 4f spins which are lattice activated at high temperatures far above TN.

KR 4.4 Tue 10:15 BEY 118

Magnetoelectric coupling in a composite multiferroic structure revealed by Ferromagnetic Resonance — •Alexander Sukhov[1], Paul P. Horley[2], Chenglong Jia[3], and Jamal Berakdar[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle/Saale, GERMANY — [2]Centro de Investigacion Materiales Avazados, S.C. (CIMAV), Chihuahua/Monterrey, MEXICO — [3]Lanzhou University, Lanzhou, CHINA

We theoretically study [1] a thin multiferroic junction related to a barium titanate (tetragonal or rhombohedral phase) layer in contact with an iron layer. Depending on the type of the magnetoelectric coupling at the interface - either due to screening charge or due to an epitaxial strain resulting in a strong magnetoelastic coupling - we present a detailed analysis of the response of the multiferroic structure to magnetic radio-frequency fields by means of ferromagnetic resonance as a function of the applied electric field.

[1] A. Sukhov, P.P. Horley, C.-L. Jia, J. Berakdar, J. Appl. Phys. **113**, 013908 (2013).

KR 4.5 Tue 10:30 BEY 118

Magnetoelectric monopoles in bulk periodic solids — •Michael Fechner[1], Eric Bousquet[1], Alexander Balatsky[2], Nicoal A. Spaldin[1], and Lars Nordström[3] — [1]ETH Zürich, Department for Materials Theory, Zürich, Switzerland — [2]NORDITA, KTH Royal Institute of Technology and Stockholm University, Stockholm, Sweden — [3]Department of Physics and Astronomy, Uppsala University, Sweden

The magnetoelectric (ME) response is described by a second rank tensor that can be decomposed into irreducible isotropic diagonal, antisymmetric and trace-free part. Here we show that the former component can be identified with a ferroic ordering of magnetoelectric monopoles[1]. We further develop a scheme to calculate the ME monopole in bulk periodic solids, by exploiting similarities to the ferroelectric polarization. Finally, as an example we present results for the series of lithium transition metal phosphate compounds ($LiMPO_4$, with M = Co, Fe and Ni), which include both ferromonopolar and antiferromonopolar ordered cases. We predict for the latter case a q-dependent diagonal ME effect.

[1] N . A. Spaldin et al., PRB 88, 094429 (2013)

KR 4.6 Tue 10:45 BEY 118

Different routes for enhanced control of ferroelectric polarization by magnetic field — •I. Fina[1,2], V. Skumryev[3,4], D. O'Flynn[5], G. Balakrishnan[5], N. Dix[2], J. M. Rebled[2,6], P. Gemeiner[7], X. Marti[8], F. Peiró[6], B. Dkhil[7], F. Sánchez[2], L. Fàbrega[2], and J. Fontcuberta[2] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Institut de Ciència de Materials de Barcelona, Catalonia, Spain — [3]Institució Catalana de Recerca i Estudis Avançats (ICREA), Catalonia, Spain — [4]Universitat Autònoma de Barcelona, Barcelona, Spain — [5]University of Warwick, Coventry, United Kingdom — [6]LENS - MIND/IN2UB, Barcelona, Spain — [7]Propriétés et Modélisation des Solides, Paris, France — [8]Faculty of Mathematics and Physics, Praha, The Czech Republic

I will focus on the direct magnetoelectric effect, control of polarization vector by magnetic field, in single-phase and composite multiferroic materials in thin film form.

In single-phase multiferroic materials, cycloidal magnet, we will see that strong coexistence of polar and non-polar regions allow large susceptibilities leading to a full control of the polarization vector by means of magnetic field [1]. In composite materials, ferromagnetic-ferroelectric heterostructures, the limiting factor is the substrate clamping effect. We will show that we can overcome this undesired effect, enhancing the presence of some small quantity of defects. These defects store the needed elastic energy, enhancing the magnetoelectric coupling, which result in huge effects near room temperature [2].

[1] I. Fina, et al., Phys. Rev. B 88, 100403(R) (2013). [2] I. Fina, et al., Nanoscale 5, 8037 (2013).

15 min. break

KR 4.7 Tue 11:15 BEY 118

Investigation of A-site Bismuth based double perovskites as potential room-temperature multiferroics — •Vikas Shabadi, Mehran VafaeeKhanjani, Mehrdad BaghaieYazdi, Aldin Radetinac, Philipp Komissinskiy, and Lambert Alff — Institute of Materials Science, Technische Universität Darmstadt, Germany

A-site Bismuth based double perovskites ($Bi_2BB'O_6$), where ferroelectricity arises from the stereochemically active $6s^2$ lone pair of electrons on the Bi^{3+} cations, provide a vital test bed to engineer room temperature multiferroicity. Here, different combinations of 3d-3d or 3d-5d cations may be introduced at the B-site in order to obtain an effective ferri/ferromagnetic moment. The 3d-3d compound Bi_2FeCrO_6 (BFCO) has drawn a heightened interest due to its large experimentally reported ferroelectricity and divergent observations of its magnetic properties. We report epitaxial BFCO thin films grown by pulsed laser deposition on single crystal $SrTiO_3(100)$ substrates. Detailed structural characterization was performed by X-ray Diffraction and the magnetic properties were studied with a SQUID magnetometer. We show that BFCO adopts a superstructure with the same unit cell as the chemically ordered double perovskite. The magnetization is a function of chemical but not of structural order.

KR 4.8 Tue 11:30 BEY 118

Room temperature magnetism and ferroelectricity in eps-Fe2O3 thin films — •I. Fina[1], M. Gich[2], A. Morelli[1], F. Sánchez[2], M. Alexe[1], J. Fontcuberta[2], and A. Roig[2] — [1]Max Planck Institute of Microstructure Physics D-06120 Hallle/Salle, Germany — [2]Institut de Ciència de Materials de Barcelona ICMAB, Consejo Superior de Investigaciones Científicas CSIC, Campus UAB 08193 Bellaterra, Catalonia, Spain

The quest for magnetoelectric multiferroics is driven by the promise of a novel generation of devices combining the best characteristics of ferromagnetic and ferroelectric materials. These cherished applications require materials displaying a substantial magnetization and electric polarization which are coupled and coexist well above room temperature. These properties are not commonly fulfilled by single phase materials and firm candidates for the development of these technologies are still sought.

In this contribution, we will report on epitaxial eps-Fe2O3 thin films grown by Pulsed Laser Deposition on (111) SrTiO3 and present recent data on its structural, magnetic and dielectric characterization. The films are ferromagnetic and ferroelectric at room temperature and display magnetization and polarization values at remanence of about 50 emu/cm3 and 1 uC/cm2 with a long retention. A magnetocapacitive response has also been detected indicating that the films present coupling between both ferroic orders.

KR 4.9 Tue 11:45 BEY 118

Time-resolved analysis of switching in spiral multiferroics — •Jonas Stein[1], Tobias Cronert[1], Jeannis Leist[2], Karin Schmalzl[3], A Agung Nugroho[4], Alexander C Komarek[5], Götz Eckold[2], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Physikalische Chemie, Universität Göttingen — [3]JCNS at ILL, France — [4]Institut Teknologi Bandung, Indonesia — [5]MPI für chemische Physik fester Stoffe

Multiferroic crystals are promising materials for future memory devices with extremely low power consumption. The rise time between two states is a crucial parameter for a possible application and was investigated in the spiral spin multiferroic $TbMnO_3$. Polarized neutron diffraction is able to determine the ratio of chiral domains, which can be controlled by an external electric field. Using the stroboscopic technique we can follow the reversion of chiral domains in the timescale of a few 100 microseconds to hours. In $TbMnO_3$ we find a clear logarithmic relation between the rise time and temperature that is fulfilled over 5 decades.

KR 4.10 Tue 12:00 BEY 118

Thermodynamic properties of the new multiferroic material $(NH_4)_2[FeCl_5(H_2O)]$ — •Matthias Ackermann[1], Daniel Brüning[2], Thomas Lorenz[2], Petra Becker[1], and Ladislav Bohatý[1] — [1]Institut für Kristallographie, Universität zu Köln, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Germany

Multiferroic materials with coupled ferroelectric and (anti-)ferromagnetic order in the same phase have attracted considerable interest during the last decade. The search for new multiferroic materials is an important issue to further improve the understanding of the underlying coupling mechanisms. Here, we present a detailed investigation of the new multiferroic compound $(NH_4)_2[FeCl_5(H_2O)]$ [1]. Our measurements of pyroelectric currents reveal, that the electric polarization occuring in the antiferromagnetically ordered phase can drastically be influenced by applying magnetic fields. Based on the results of these dielectric investigations, together with measurements of thermal expansion, magnetostriction and specific heat, detailed magnetic field versus temperature phase diagrams are derived. Depending on the direction of the magnetic field up to three different multiferroic phases are identified, which are separated from the paramagnetic phase by a magnetically ordered, but non-ferroelectric phase.

This work was supported through the Institutional Strategy of the University of Cologne within the German Excellence Initiative.

[1] Ackermann M et al. 2013 *New J. Phys.* (in press, arXiv:1308.0285)

KR 4.11 Tue 12:15 BEY 118

Stoichiometric Effects on Crystal Quality in $LuFe_2O_4$ and $YbFe_2O_4$ — •Hailey Williamson[1,2], Geetha Balakrisnan[2], and Manuel Angst[1] — [1]Jülich Centre for Neutron Science JCNS-2 and Peter Grünberg Institut PGI-4, Forschungszentrum Jülich GmbH, Jülich, Germany. — [2]Department of Physics, The University of Warwick, CV4 7AL, Coventry, UK

The multiferroic rhombohedral $LnFe_2O_4$ (Ln=Lu, Y, Yb, Tm, Ho and Er) system, which can be described as stacked hexagonal Fe bilayers separated by Lu monolayers, has been in focus since the discovery of

interesting magnetic and electrical characteristics in $LuFe_2O_4$. The specific CO configuration within the Fe bilayers was initially thought to produce a ferroelectricity through cross polarization of the two layers of the bilayer. However our recent investigations indicate that the CO configuration is actually non-polar. Extensive research highlighted a large sensitivity to oxygen stoichiometry, where crystals grown in an excess/deficient oxygen partial pressure environment exhibit smeared glassy magnetic transitions and diffuse CO. Through fine tuning of the atmospheric conditions, crystals exhibiting 3D CO and magnetism were produced. Interest then spread to isostructural $YbFe_2O_4$, which has currently few detailed investigations. Single crystals of $YbFe_2O_4$ were grown in four different partial pressure atmospheres to view the effects of oxygen stoichiometry on the magnetism and CO. A series of macroscopic and microscopic measurements provided a detailed look into the effects of oxygen stoichiometry on the intrinsic characteristics as well as a comparison to that of its predecessor $LuFe_2O_4$.

KR 4.12 Tue 12:30 BEY 118

Multiferroicity in Cu_2OSeO_3? — •Eugen Ruff[1], Stephan Krohns[1], Helmuth Berger[2], Peter Lunkenheimer[1], and Alois Loidl[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg — [2]Institute of Physics of Complex Matter, École Polytechnique Fédérale de Lausanne

Skyrmions are topologically stable vortex-like objects, for the first time detected in the B20 alloy MnSi [1]. Their electrical controllability via small currents qualifies skyrmions for applications in high-density magnetic storage devices. The recent discovery of magnetoelectric skyrmions in the insulating chiral magnet Cu_2OSeO_3 leads to another promising route to electrical control [2]. This system is suggested to carry a local electrical dipole, which implies that the skyrmions should be controllable by an external electrical field without losses due to Joule heating. Here we provide a thorough analysis of the magnetic and polar phases of this material, using SQUID and pyrocurrent measurements. In order to investigate the possible ferroelectric properties of Cu_2OSeO_3, we have performed dielectric spectroscopy in various magnetic fields in a broad frequency range below 70 K. Combining all these different techniques, we address the question whether Cu_2OSeO_3 is magnetoelectric or multiferroic. [1] S.Mühlbauer *et al.*, Science **323**, 915 (2009). [2] S.Seki *et al.*, Science **336**, 198 (2012).

KR 5: Multiferroics II (MA jointly with DF, DS, KR, TT)

Time: Wednesday 9:30–13:00 Location: HSZ 04

KR 5.1 Wed 9:30 HSZ 04

An Engineered Polar Oxide Heterostructure Built from Isosymmetric Magnetically Ordered Components — •Matthew S Dyer[1], Jonathan Alaria[1], Pavel Borisov[1,5], Troy D Manning[1], Serban Lepadatu[2], Markys G Cain[2], Elena D Mishina[3], Natalia E Sherstyuk[3], N A Ilyin[3], Joke Hadermann[4], David Lederman[5], John B Claridge[1], and Matthew J Rosseinsky[1] — [1]University of Liverpool, Liverpool, UK — [2]National Physical Laboratory, Teddington, UK — [3]Moscow State Technical University, Moscow, Russia — [4]University of Antwerp, Antwerp, Belgium — [5]West Virginia University, Morgantown, USA

Theory predicts that certain layered heterostructures consisting of perovskite blocks have non-centrosymmetric structures. The breaking of spatial inversion symmetry arises through a combination of octahedral tilting and A site ordering. Following this prediction, we grow a thin-film of the $[(YFeO_3)_5(LaFeO_3)_5]_{40}$ heterostructure using RHEED monitored pulsed layer deposition. Polar domains are present in the thin-film, as demonstrated by second harmonic generation and piezoelectric force microscopy measurements. We experimentally confirm that the heterostructure is also magnetically ordered at room temperature with a finite magnetization, retaining the magnetic structure of the individual $YFeO_3$ and $LaFeO_3$ components.

KR 5.2 Wed 9:45 HSZ 04

First-principles study of the $BaTiO_3/BaFeO_3$ perovskite interface — •Igor Maznichenko[1], Sergey Ostanin[2], Arthur Ernst[2], and Ingrid Mertig[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Epitaxial growth can combine a robust ferroelectric, such as $BaTiO_3$, and strong ferromagnets into the so called composite multiferroic films. The switching properties of artificial multiferroics sandwiched between metallic contacts make them excellent candidates for the room temperature four-state memories.

Regarding the ferromagnetic side of composite multiferroics, we suggest to use the cubic perovskite $BaFeO_3$ whose epitaxial growth has been recently reported. Here, from the basis of *ab-initio* electronic structure calculations, within the Korringa-Kohn-Rostoker method, we study the magnetic properties of bulk $BaFeO_3$. The approach allows us to accurately monitor the evolution of the Curie temperature upon both the tetragonal distortions and presence of oxygen vacancies. Finally, we examine magnetoelectricity at the $BaTiO_3/BaFeO_3$ interface.

KR 5.3 Wed 10:00 HSZ 04

Behaviour of Raman modes in $BiFeO_3$ epitaxial thin films with respect to azimuthal orientation — •Andreas Talkenberger[1], Cameliu Himcinschi[1], Ionela Vrejoiu[2,3], Florian Johann[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, Leipziger Str. 23, D-09596 Freiberg, Germany — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany — [3]Max Planck Institute for Solide State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany

$BiFeO_3$ (BFO) is an interesting candidate for multiferroic applications. In this work we focus on the Raman spectroscopic investigation of epitaxially grown thin films of BFO by pulsed laser deposition on different substrates, belonging to the group of scandates ($DyScO_3$, $SmScO_3$, $GdScO_3$). The Raman spectra were recorded using the 442 nm emission line of a He-Cd laser. Some phonon modes show changes in the position, full width at half maximum (FWHM) and intensity depending on the azimuthal angle. We found a 90 degree periodicity of the peak position and of the FWHM for particular modes. For both parallel and crossed polarisation the four maxima in positions correspond to the minima in FWHM. Such a behaviour can be explained considering a twin family of domains with a very well defined orientation to each other. Our results are supported by piezoresponse-force microscopy and X-ray diffraction measurements as well.

KR 5.4 Wed 10:15 HSZ 04

$BiFeO_3/LaFeO_3$: a magnetoelectric multiferroic — •Zeila Zanolli[1,3], Jacek Wojdel[2], Jorge Iniguez[2], and Philippe Ghosez[3] — [1]Forschungszentrum Jülich, PGI and IAS, Jülich, Germany — [2]ICMAB-CSIC, Bellaterra, Spain — [3]Université de Liège, Physics Department, Lieǵe, Belgium

Transition-metal oxides of perovskite structure present a wide variety of physical properties. In particular, there is a strong interest in multiferroic materials that are simultaneously ferroelectric and magnetic (*magnetoelectrics*). Due to the scarcity of natural magnetoelectric multiferroics and thanks to recent advances in epitaxial growth techniques, designing new magnetoelectric multiferroic heterostructures is a promising way to succeed in this quest.

First-principles techniques are used to investigate electric control of the magnetization in the $BiFeO_3/LaFeO_3$ perovskite oxide superlattice (SL) on a (001)-$SrTiO_3$ substrate. Our results [1] show that the $BiFeO_3/LaFeO_3$ SL exhibits a trilinear coupling of a polar mode with two different rotations of the oxygen cages (*hybrid improper ferroelectricity*). Non-collinear spin calculations reveal that the ferroelectric ground state also presents weak ferromagnetism with easy axis along the [1 -1 0] direction. The microscopic mechanism allowing one to manipulate the magnetization with an electric field in such systems is presented and its dependence on strain and chemical substitution is discussed. The $BiFeO_3/LaFeO_3$ SL is found to be a good candidate to attain electric switching of magnetization at room temperature.

[1] Phys. Rev. B **88**, 060102(R) (2013)

KR 5.5 Wed 10:30 HSZ 04

The influence of strain on the optical properties of pseudo-tetragonal $BiFeO_3$ thin films — •Cameliu Himcinschi[1], Akash Bhatnagar[2], Andreas Talkenberger[1], Dietrich R.T. Zahn[3], Jens

Kortus[1], and Marin Alexe[2,4] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09596 Freiberg, Germany — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany — [3]Semiconductor Physics, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [4]Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom

Tetragonally distorted $BiFeO_3$ recently attracted a lot of attention because of its interesting multiferroic properties and the larger spontaneous polarization as compared to its rhombohedral counterpart. Highly strained (when grown on $LaAlO_3$ substrates) and nearly pseudomorphic (when grown on $TbScO_3$ substrates) $BiFeO_3$ films were deposited by pulsed laser deposition. The symmetry of the tetragonally distorted $BiFeO_3$ films is discussed based on polarisation dependent Raman measurements and the comparison with Raman spectra measured for films deposited on $TbScO_3$. The evaluation of ellipsometric spectra reveals that the films deposited on $LaAlO_3$ are optically less dense and the dielectric function is blue-shifted by more than 0.3 eV as compared to the films deposited on $TbScO_3$. By analyzing the absorption edge using a bandgap model, bandgaps of 3.10 eV and 2.75 eV were determined for the films deposited on $LaAlO_3$ and $TbScO_3$, respectively. This work is supported by the German Research Foundation DFG HI 1534/1-1.

KR 5.6 Wed 10:45 HSZ 04

Electrically induced magnetic transiton at the LSMO/BTO interface — •Markus Schmitz, Alexander Weber, Paul Zakalek, Markus Waschk, and Thomas Brückel — Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich Germany

The magnetoelectric coupling is one of the most fascinating and active research areas today. The control of the magnetism due to an applied electric field may lead to new device concepts. First principles calculations of $La_{(1-x)}Sr_xMnO_3/BaTiO_3(001)$ interfaces show magnetic reconstructions due to the change of the polarization of BTO by applying an external electric field. The different electron densities influence the equilibrium between super- and double-exchange favoring a ferromagnetic or an antiferromagnetic order at the interface for the two different orientations of the polarization. Here we report on LSMO/BTO, grown with an Oxide Molecular Beam Epitaxy system. The epitaxial layer-by-layer growth was confirmed by in-situ RHEED analysis and the crystalline quality of the surface was investigated by LEED and Atomic Force Microscopy. The structural characterization was carried out by X-ray reflectometry and diffraction. We could prove the possibility to electrically polarize $BaTiO_3$ substrates due to an applied voltage of 400V by optical methods. The macroscopic magnetic properties were determined by MOKE and SQUID magnetometry. The magnetic formation at the interface with respect to the polarization of the $BaTiO_3$ was investigated by Polarized Neutron reflectometry measurements performed at MARIA (FRM II).

15 min. break

KR 5.7 Wed 11:15 HSZ 04

Growth and structure characterization of double perovskite Sr2FeMoO6 thin films — •Hakan Deniz[1], Dietrich Hesse[1], Marin Alexe[1], Robert Lowndes[2], and Lucian Pintilie[2] — [1]Max-Planck Institute of Microstructure Physics, Weinberg 2, D-06120, Halle (Saale), Germany — [2]National Institute of Materials Physics, Atomistilor 105bis, Magurele 077125, Romania

The double perovskite Sr2FeMoO6 (SFMO) has drawn considerable attention recently owing to some of its unique features such as high Curie temperature (˜410K) and half-metallic ferrimagnetic nature with a high saturation moment of 4μB. The low-field room temperature magnetoresistance observed in SFMO makes it an attractive candidate for oxide spintronics applications. However, the broad distribution of results reported so far on SFMO films suggests that an optimal structure is attainable only within a narrow window of growth conditions; and magnetic/transport properties are highly akin to Fe and Mo atomic site disorder. Pulsed laser deposition was employed to grow SFMO thin films on vicinal SrTiO3 substrates from a custom-made stoichiometric target using argon as ambient gas. X-ray diffraction data revealed that the SFMO films were grown epitaxially with respect to the substrate, including, however, a small percentage of secondary phases. The morphology of the films shows flat plains with embedded grain- or needle-like structures, which are most likely the result of spurious phases. The nature of these defects and their interfaces with the SFMO matrix are under investigation by transmission electron microscopy. This work is supported by the EU-FP7 project IFOX.

KR 5.8 Wed 11:30 HSZ 04

Magnetic Anisotropy in Multiferroic Lu_2MnCoO_6 — •Martin Lonsky[1], Merlin Pohlit[1], María Antonia Señarís Rodríguez[2], and Jens Müller[1] — [1]Physikalisches Institut, Goethe-Universität, Frankfurt (M), Germany — [2]Dpto. Química Fundamental U. Coruña, Coruña, Spain

Lu_2MnCoO_6 recently has been introduced as a new type-II multiferroic with ferroelectricity due to charge ordering and magnetostriction related to magnetic Mn^{4+} and Co^{2+} ions which are arranged alternately in the form of Ising chains along the c-axis of the crystal [1]. The magnetic properties, however, remain puzzling, which in particular is due to the lack of measurements on single crystals, that have not yet successfully been synthesized. Here, we present for the first time measurements of the magnetic anisotropy by employing micro-Hall magnetometry on a few micrograins of dimensions $\sim 1\,\mu$m only. Our results reveal a strong dependence of magnetic hysteresis on temperature and the applied field direction. This anisotropy is also reflected in the observation of a variety of unusual effects as for instance wasp-waisted hysteresis loops, sharp jumps in magnetization at about $T = 300\,$mK and an exchange bias, ocurring in each case in only one field direction. Additionally, the observation of a pronounced maximum in the coercive field at $T_{SF} \sim 12\,$K indicates a significant change in the spin dynamics of the system below T_{SF}, similar to the behavior of the related compound $Ca_3Co_{2-x}Mn_xO_6$ ($x \approx 0.95$) [2].

[1] S. Yáñez-Vilar et al., Phys. Rev. B. 84, 134427 (2011).
[2] T. Lancaster et al., Phys. Rev. B 80, 020409 (2009).

KR 5.9 Wed 11:45 HSZ 04

The multiferroic $CuCrO_2$ compound: interlayer exchange and domain population — •Matthias Frontzek — Laboratory for Neutron Scattering, Paul Scherrer Institut, 5232 Villigen-PSI, Switzerland

Multiferroic materials have become of interest for their unusual low-temperature properties in general, and the tunability of the magnetic structure through an electric field and the electric polarization through a magnetic field in particular. The most promising candidates for such controllable multiferroics have been found among the materials with inherent geometric magnetic frustration.

Among these, the delafossite $CuCrO_2$, which crystallizes in the rhombohedral $R\bar{3}m$ space group, is a multiferroic compound with an apparent strong coupling of spin and charge. In contrast to other multiferroic compounds $CuCrO_2$ shows a spontaneous electric polarization upon antiferromagnetic ordering without an accompanying structural phase transition, thus the magnetic ordering alone breaks the inversion symmetry. The peculiar magnetic structure of $CuCrO_2$ allows the direct quantitative analysis of the domain population.

In our contribution, we present a detailed study on $CuCrO_2$ single crystals using neutron diffraction in applied electric and magnetic fields. With the fields we were able to tune the multiferroic states in $CuCrO_2$ and could directly relate them to the underlying domain physics. Our results allow the re-interpretation of macroscopic measurements and show that the $p-d$ hybridization is the dominant spin-charge coupling mechanism.

KR 5.10 Wed 12:00 HSZ 04

Structure and Magnetic Coupling in $YBaFeCuO_5$ — •Andrea Scaramucci[1], Mickael Morin[2], Ekaterina Pomjakushina[2], Marek Bartkowiak[2], Denis Sheptyakov[2], Lukas Keller[2], Juan Rodriguez-Carvajal[3], Michel Kenzelmann[2], Kazimierz Conder[2], Marisa Medarde[2], and Nicola A. Spaldin[1] — [1]Materials Theory, ETH-Zurich, Zurich, Switzerland — [2]Paul Scherrer Institute, Villigen, Switzerland — [3]Institute Laue Langevin, Grenoble, France

We theoretically study the structure and exchange couplings in multiferroic $YBaFeCuO_5$ (YBFCO). Using density functional theory we calculate energies of configurations with various Fe^{3+}/Cu^{2+} orderings in the bilayered perovskite structure of YBFCO. We find that configurations with different distribution of Fe^{3+} and Cu^{2+} ions fall into two groups with distinctly different energies. The energies of those in the lowest energy group are close to that of the ground state (relative to the growth temperature) suggesting Fe^{3+} and Cu^{2+} to be disordered in YBFCO. Finally, we calculate exchange coupling constants for all the low energy configurations and show that the magnetic ordering resulting from these couplings is compatible with the experimentally-observed high-temperature magnetic ordering. However, they do not

explain the existence of the experimentally observed low-temperature incommensurate magnetic structure.

KR 5.11 Wed 12:15 HSZ 04

Hybrid-functional study of the structural, magnetic and electronic properties of rare-earth nickelates — •Konstantin Z. Rushchanskii, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Rare-earth nickelates ($ReNiO_3$) are very promising functional perovskite crystalline materials, exhibiting metal-insulator (MI) transition, which can be continuously controlled by composition, bi-axial strain and(or) electric field. Unfortunately, conventional *ab initio* DFT+U results fail to reproduce their magnetic ground state as well as the effect of epitaxial strain on MI transition temperature. We present results of our comprehensive study of structural, magnetic and electronic properties of bulk $ReNiO_3$ (Re=Y, Gd, Eu, Sm, Nd and Pr) and strained $SmNiO_3$ films [1], performed with HSE06 functional. We show correlation between MI transition temperature and structural parameters of bulk and films, which nicely fits known experimental data. We also analyze the difference in the electronic structure obtained in DFT+U and with the hybrid functional and their influence on the resulting magnetic ordering in the ground state.

We acknowledge the support by Helmholtz Young Investigators Group Programme VH-NG-409, JSC and JARA-HPC.

[1] F.Y. Bruno, K.Z. Rushchanskii, S. Valencia, Y. Dumont, C. Carrétéro, E. Jacquet, R. Abrudan, S. Blügel, M. Ležaić, M. Bibes, and A. Barthélémy, Phys. Rev. B 88, 195108 (2013).

KR 5.12 Wed 12:30 HSZ 04

Magnetic properties of multiferroic $TbMnO_3$ — •Natalya Fedorova, Andrea Scaramucci, Claude Ederer, and Nicola Spaldin — ETH Zurich, Materials Theory, Wolfgang-Pauli-Strasse 27, CH-8093 Zurich, Switzerland

We use ab-initio calculations to investigate the magnetic properties of multiferroic $TbMnO_3$.

At low temperatures $TbMnO_3$ demonstrates an incommensurate spiral ordering of Mn spins which is accompanied by appearance of spontaneous electric polarization driven by applied magnetic field [1]. The establishment of such spin ordering is usually described within the framework of a Heisenberg model with competing nearest-neighbor and next-nearest-neighbor exchange interactions. However, our theoretical estimations of these interactions by ab-initio calculations demonstrate a clear deviation from Heisenberg model.

We consider first the coupling between magnetic and orbital orderings as a main source of non-Heisenberg behavior in $TbMnO_3$, but conclude that it does not explain the observed deviation. We find that higher order interactions (biquadratic and four-body spin couplings) should be taken into account for proper treatment of the magnetism in $TbMnO_3$.

[1] T. Kimura et al., Nature 426, 55-58 (2003)

KR 5.13 Wed 12:45 HSZ 04

Coupling of epitaxial strain and point-defect formation in perovskites — •Ulrich Aschauer, Philipp Baumli, and Nicola A. Spaldin — Materials Theory, ETH Zurich, Zürich, Switzerland

Using density functional theory calculations we recently established the existence of a strong coupling between epitaxial strain and the formation energy of oxygen vacancies in the model perovskite $CaMnO_3$ (Phys. Rev. B. 88, 054111, 2013). Here we investigate the generality of this concept for other oxides including metallic perovskites and also investigate the effect of strain on the formation of cation vacancies. We find that in general the response of the defect profile follows the behavior expected from chemical-expansion arguments, with tensile strain favoring oxygen vacancies and compressive strain favoring cation vacancies. We show, however, that material-specific details of the electronic structure can cause deviations from this trend under both tensile and compressive strain.

KR 6: Invited Talk - Stefan Förster (DF jointly with O, DS, KR, MM)

Time: Wednesday 10:30–11:15 Location: GER 37

Invited Talk KR 6.1 Wed 10:30 GER 37

Two-dimensional Oxide Quasicrystals: A new class of materials? — •Stefan Förster[1], Klaus Meinel[1], Rene Hammer[1], Martin Trautmann[1], and Wolf Widdra[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

Two-dimensional materials - like graphene, hexagonal boron nitride, or topological insulators - have recently pioneered a new field of materials science. Their peculiar properties are often related to their specific two-dimensional periodic structure.

Here we report the first observation of a two-dimensional oxide quasicrystal (QC), a new member in the family of 2D materials [1]. The QC is derived from $BaTiO_3$ thin films on a hexagonal Pt(111) substrate. Low-energy electron diffraction (LEED) reveals a twelve-fold rotational symmetry. Scanning tunneling microscopy (STM) at room temperature as well as at low temperatures (80 K) allow to resolve the atomic structure. The aperiodic structure is formed by primitive atomic arrangements in squares, triangles, and rhombi with a universal edge length of 0.69 nm. In addition to this dodecagonal atomic arrangement, building blocks of squares, triangles,and rhombi are also found on $(2+\sqrt{3})$ and $(2+\sqrt{3})^2$ larger scales indicating the characteristic self-similarity of an ordered QC. The observed interface-driven formation of a 2D QC from a perovskite oxide in contact with a hexagonal substrate is expected to be a general phenomenon.

[1] S. Förster, K. Meinel, R. Hammer, M. Trautmann, and W. Widdra, *Nature 502*, 215 (2013).

KR 7: Invited Talk - Heidemarie Schmidt (DF jointly with MA, HL, DS, KR)

Time: Wednesday 15:00–15:45 Location: GER 37

Invited Talk KR 7.1 Wed 15:00 GER 37

Smart multiferroic thin films for cognitive computing — •Heidemarie Schmidt — Technische Universität Chemnitz, Department of Materials for Nanoelectronics, Reichenhainer Str. 39, 09126 Chemnitz

Cognitive systems promise to penetrate complexity and assist people and organizations in better decision making [1]. We have successfully prepared metal-multiferroic-metal (MMM) structures with the multiferroic material BiFeO3 and BiFeTiO3. All those MMM structures exhibit nonvolatile resistive (meristive) switching. Investigations of memristive switching is driven by promising applications of power-efficient memristive nanostructures including data storage, logic systems, cognitive computing and artificial neural networks. Prominence of work on memristive systems might be visualized by the near-future breakthrough in computing technology, where classical Von Neumann architecture is replaced by cognitive systems. In this talk I present three new functionalities of smart MMM structures including nonvolatile multilevel resistive switching [2], nonvolatile reconfigurable logics and nonvolatile second and higher harmonics generation [3] which are very promising for the development of cognitive computing. [1] J. E. Kelly III, S. Hamm, Smart Machines: IBM*s Watson and the Era of Cognitive Computing, Columbia University Press, 2013 [2] Y. Shuai et al., J. Appl. Phys. 109 (2011); Appl. Phys. Lett. 98 (2011); Appl. Phys. Exp. 4 (2011); 111 (2012); IEEE Electron Device Letters 34 (2013); Scientific Reports 3 (2013) [3] N. Du et al., Rev. Sci. Instr. 84 (2013)

KR 8: Poster Crystallography

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

KR 8.1 Wed 17:00 P4

Analyzing high pressure diffraction data of perovskites with parametric Rietveld refinement and rotational symmetry modes of a rigid body — •Martin Etter[1], Melanie Müller[1], Michael Hanfland[2], and Robert E. Dinnebier[1] — [1]Max Planck Institut für Festkörperforschung, Stuttgart, Germany — [2]European Synchrotron Radiation Facility (ESRF), Grenoble, France

The high pressure behavior of crystals can best be observed with X-ray or neutron diffraction methods, as these methods allow the application of least square iteration processes (e.g. Rietveld method) to refine parameters, which are directly connected with structural and/or magnetic changes within the crystal. A challenge of the investigation of diffraction patterns under high pressure is that the data quality often decreases after only a few GPa, which makes it difficult for a least square iteration process to find the correct minimum. For this reason, adequate structural models are needed in order to stabilize the refinement and to decrease the number of free parameters. Such models can be provided by the application of rigid bodies, symmetry modes or the recently developed method of rotational symmetry modes of a rigid body which combines the advantages of both. Additionally, these models can be parameterized, treating different data sets simultaneously with the application of physical equations as constraints, which leads to a further reduction of refined parameters. In order to illustrate the power of this new approach, sequential and parametric Rietveld refinements of a LaFeO3 perovskite investigated with synchrotron powder X-ray diffraction under high pressure were carried out.

KR 8.2 Wed 17:00 P4

Using an innovative Vinet EoS approximation for parametric refinement of high pressure powder diffraction data — •Martin Etter and Robert E. Dinnebier — Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

The relationship between the thermodynamic state variables pressure, volume and temperature can normally be described with so-called equation of states (EoS), which are semi-empirical determined and which are often used with an isothermal description. Among this semi-empirical EoS, the Vinet EoS is believed to be the most accurate, allowing to describe the behavior of most material systems under high pressure up to a compression of 40%. Similar to other EoS like the Birch-Murnaghan EoS or the natural strain EoS, the Vinet EoS has an pressure on volume dependency, which makes it unsuitable for parametric refinement of high pressure powder diffraction data, where the pressure is the independent variable and the volume is the dependent which is a refineable quantity. Using an innovative Taylor series expansion of the Vinet EoS, it is possible to obtain an equation which is analytical invertible and therefore useful for a direct parametric refinement in analysis programs like TOPAS. By means of high pressure powder diffraction data of different material systems the validity of the newly developed EoS is evaluated and demonstrated.

KR 8.3 Wed 17:00 P4

Crystallografic orientation of hydrogen defects in lithium niobate and lithium tantalate — •Thomas Köhler, Erik Mehner, Juliane Hanzig, Günter Gärtner, Hartmut Stöcker, and Dirk C. Meyer — Institut für Experimentelle Physik, Technische Universität Bergakademie Freiberg, D-09596 Freiberg, Germany

Pyroelectric crystals are used in many optical devices, therefore, understanding the structural defects is helpful to control optical and electrical properties. It is easy to incorporate hydrogen in air-grown $LiNbO_3$ and $LiTaO_3$ crystals, however, the exact processes are only partially understood. The incorporation of hydrogen in the two materials is investigated crystal axis resolved and polarization-dependent by FT-IR spectroscopy. In the congruent material systems the hydrogen defect causes an OH band with several sub-bands, at different spectral positions for both materials.

The examined congruent crystals are cube shaped, cut and polished along the [001], [100] and [110] directions. The OH band show a significantly weaker signal for the [100] and [110] directions than for the [001] direction of the crystal cubes. Further measurements were made in the far infrared range. The aim of the crystal axis resolved and polarization-dependent study is the development of a structural model for the orientation of the OH defects of the two pyroelectric materials.

KR 8.4 Wed 17:00 P4

Transmission Kikuchi Diffraction and Selected Area Electron Diffraction studies of WS_2 nanotubes — Andrey Chkanov[1], Azat Khadiev[1], •Nathanael Jöhrmann[2], Dmitry Pashin[1], and Michael Hietschold[2] — [1]Kazan National Research Technical University named after A.N. Tupolev, Nanotechnology in Electronics Department, Kazan, Russia — [2]Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

Investigations of nanotubes have shown that tubes may differ not only in chemical composition but also in structure. Selected area electron diffraction (SAED) in TEM is a well-established method that allows distinguishing structural parameters of single nanotubes. However in the case of single tubes deposited on a bulk substrate TEM methods do not work. An alternative might be electron backscatter diffraction (EBSD). Clear understanding of peculiarities of Kikuchi diffraction found on nanotubes requires comparative studies. Using SAED and transmission Kikuchi diffraction (TKD) allows a comparison between a SAED pattern and an EBSD like Kikuchi diffraction pattern obtained from one and the same tube lying on a TEM grid.

We combine SAED and TKD measurements with pattern simulations for structural analysis of WS_2 nanotubes. SAED studies allowed determining parameters of the unit cell and chiral angle of the tube. In the TKD studies a peculiar intense band was observed for most nanotubes, which might also contain information about the chiral angle. In some cases two TKD patterns seemed to overlap. Structure models were proposed to explain this effect.

KR 8.5 Wed 17:00 P4

Combining SAXS and TEM to reveal the mechanism of nucleation and growth of anisotropic noble metal nanoparticles — •Tilo Schmutzler, Torben Schindler, Martin Schmiele,

Thaer Kassar, Christian Bär, and Tobias Unruh — Chair for Chrystallography and Structural Physics, Friedrich-Alexander University Erlangen-Nürnberg, Staudtstr. 3, 91058 Erlangen, Germany

Anisotropic noble metal nanoparticles like nanorods or nanowires of gold and silver have been the subject of widespread research in the last two decades because of their possible applications i.e. in biological imaging and drug delivery. One common synthesis is the seed-mediated growth method, where a noble metal precursor is reduced in aqueous solution to form isomorphic seed particles that lead to anisotropic nanorods by further reduction of the precursor in the presence of cetyltrimethylammonium bromide (CTAB). Neither the exact formation mechanism of the seed particles nor that of the anisotropic growth in the presence of CTAB is completely understood up to now.

In situ time-resolved small angle x-ray scattering (SAXS) is a powerful tool to study the size and shape of nanoparticles in dependence of temperature and time during their formation and growth. In addition, transmission electron microscopy (TEM) reveals the current shape, polydispersity and size distribution of the particles. In the poster we will present studies to reveal the mechanism of nucleation and growth of anisotropic noble metal nanoparticles under the load of CTAB combining the results of the complimentary techniques of in situ SAXS and ex situ TEM.

KR 9: Recent Developments in X-ray Diffraction

Time: Thursday 10:15–11:00 Location: CHE 184

KR 9.1 Thu 10:15 CHE 184

A diffraction effect in X-ray area detectors — •Christian Gollwitzer and Michael Krumrey — Physikalisch-Technische Bundesanstalt, Berlin, Germany

When an X-ray area detector with a single-crystalline sensor layer, such as a hybrid pixel detector, is used to record a scattering or diffraction image, a pattern of lines can appear which overlays the detected images.[1] This pattern with an intensity decrease of up to 20% is caused by diffraction in the sensor layer. Experimental images of a modular PILATUS 1M detector[2] together with a theory are presented over a photon energy range from 3.4 keV to 10 keV. The effect can be exploited to measure the photon energy of the beam and angular misalignment of the detector.

[1] C Gollwitzer & M Krumrey: *A diffraction effect in X-ray area detectors*, submitted to *J. Appl. Cryst.* (2013) `arXiv:1308.6525`

[2] J Wernecke, C Gollwitzer, P Müller & M Krumrey: *Characterization of an in-vacuum PILATUS 1M detector*, submitted to *J. Synchrotron Rad.* (2013) `arXiv:1311.5082`

KR 9.2 Thu 10:30 CHE 184

Beam Conditioning in Cutting Edge X-ray Analytical Equipment — •Jörg Wiesmann, André Beerlink, Andreas Kleine, Jürgen Graf, Frank Hertlein, and Carsten Michaelsen — Incoatec GmbH, Geesthacht

Nowadays, X-ray optical components, such as multilayer mirrors or scatterless apertures, are used as beam conditioning devices in nearly all state-of-the-art X-ray analytical equipment.

Scatterless apertures, such as the scatterfree pinholes SCATEX, are usually made of oriented single crystals, and enable a beam conditioning that is free of parasitic scattering commonly associated with conventional metal apertures. Therefore, such pinholes allow a significant improvement of small angle scattering instruments as the number of necessary pinholes can be reduced while simultaneously enlarging the beam defining pinhole size. This leads to an increased flux on the sample.

Multilayer X-ray mirrors are widely used as monochromators and beam shaping devices in protein and small molecule crystallography. Beam shaping with multilayer mirrors includes the optimization of the flux on the sample and the control over the beam shape and divergence.

In this contribution, we will give an overview of current developments in multilayer optics and scatterless beam components, showing their benefit for typical applications in combination with high-brightness microfocus X-ray sources. We will be presenting selected results for protein crystallography and small angle scattering obtained with the METALJET X-ray source.

KR 9.3 Thu 10:45 CHE 184

Analyzing high pressure diffraction data of perovskites with parametric Rietveld refinement and rotational symmetry modes of a rigid body — •Martin Etter[1], Melanie Müller[1], Michael Hanfland[2], and Robert E. Dinnebier[1] — [1]Max Planck Institut für Festkörperforschung, Stuttgart, Germany — [2]European Synchrotron Radiation Facility (ESRF), Grenoble, France

The high pressure behavior of crystals can best be observed with X-ray or neutron diffraction methods, as these methods allow the application of least square iteration processes (e.g. Rietveld method) to refine parameters, which are directly connected with structural and/or magnetic changes within the crystal. A challenge of the investigation of diffraction patterns under high pressure is that the data quality often decreases after only a few GPa, which makes it difficult for a least square iteration process to find the correct minimum. For this reason, adequate structural models are needed in order to stabilize the refinement and to decrease the number of free parameters. Such models can be provided by the application of rigid bodies, symmetry modes or the recently developed method of rotational symmetry modes of a rigid body which combines the advantages of both. Additionally, these models can be parameterized, treating different data sets simultaneously with the application of physical equations as constraints, which leads to a further reduction of refined parameters. In order to illustrate the power of this new approach, sequential and parametric Rietveld refinements of a LaFeO3 perovskite investigated with synchrotron powder X-ray diffraction under high pressure were carried out.

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

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

KR 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.

KR 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.

KR 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.

KR 11: Nano- and microstructured dielectrics (DF jointly with KR)

Time: Thursday 12:00–12:40 Location: GER 37

KR 11.1 Thu 12:00 GER 37

Influence of nano crystallites in barium titanate glass ceramics on the ferroelectric phase transition — •Berit Körbitzer, Martun Hovhannisyan, and Martin Letz — Schott AG, Mainz

Dielectrics based on glass ceramics with ferroelectric phases have potential for application as high power capacitors because of their intrinsic pore-free structure. Due to this property glass ceramics reach high dielectric breakdown strengths compared to conventional ceramic materials. In addition the nano cristalline structure broadens the sharp ferroelectric transitions and allows applications up to 200°C. By solid solution type doping and variation of crystallite size one can influence the ferroelectric transition temperature of barium titanate based glass ceramics. The effect of strontium and zirconium doping on the dielectric properties and glass stability of this system is analysed.

KR 11.2 Thu 12:20 GER 37

Polarization-dependent second harmonic analysis of ferroelectric domain structures in z-cut lithium niobate — •Alex Widhalm[1], Moritz Grothe[1], Gerhard Berth[1,2], and Artur Zrenner[1,2] — [1]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [2]Center for Optoelectronics and Photonics Paderborn (CeOPP), 33098 Paderborn, Germany

Short-periodic domain grids in ferroelectric materials like lithium niobate (LN) are inevitable to achieve quasi phase matching for sophisticated applications in the visible spectral range. A deeper understanding of the physical processes involved in the periodic inversion of the spontaneous dielectric polarization is essential for guaranteeing sufficient quality of these domain structures. Within this work we study the nonlinear signature of the z-cut surface region of periodically poled LN with integrated Ti waveguide structures by means of second harmonic microscopy. In this context, the polarization-dependent SH-analysis has turned out to be an extremely high contrastive method for imaging the ferroelectric domain structure. In addition this technique enables directly the assignment of polarity. All in all, it has been proven that the occurring nonlinear signatures are essentially determined by the polarization and the tailored crystal structure.

KR 12: Functional Materials - Analysis with EBSD, X-Ray Kossel Diffraction and Related Methods (MI jointly with KR)

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

Invited Talk KR 12.1 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.

KR 12.2 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.

KR 12.3 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.

KR 12.4 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.

KR 12.5 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.

KR 13: Crystallography in Materials Science (KR jointly with DF, MI)

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

Invited Talk KR 13.1 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.

KR 13.2 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).

KR 13.3 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)

KR 13.4 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

KR 13.5 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.

KR 13.6 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 Facil-

ity, 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.

KR 13.7 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).

KR 13.8 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.

KR 14: Mitgliederversammlung FG Kristallographie

Time: Thursday 17:45–18:30 Location: CHE 184

Mitgliederversammlung FG Kristallographie