Crystallography Division
Fachgruppe Kristallographie (KR)

David Rafaja
Institute of Materials Science
TU Bergakademie Freiberg
Gustav-Zeuner-Straße 5
09599 Freiberg
rafaja@ww.tu-freiberg.de

Overview of Invited Talks and Sessions

Invited talks of the joint symposium SYCE

See SYCE for the full program of the symposium.

SYCE 1.1	Mon	15:00–15:30	HSZ 02	**Ferroelectric domain walls: from conductors to insulators and back again** — •Petro Maksymovych
SYCE 1.2	Mon	15:30–16:00	HSZ 02	**Zoology of skyrmions and the role of magnetic anisotropy in the stability of skyrmions** — •Istvan Kezsmarki, Sandor Bordacs, Jonathan White, Vladimir Tsurkan, Alois Loidl, Peter Milde, Hiroyuki Nakamura, Andrey Leonov
SYCE 1.3	Mon	16:00–16:30	HSZ 02	**Magnetic imaging of topological phenomena in ferroic materials** — •Weida Wu
SYCE 1.4	Mon	17:00–17:30	HSZ 02	**Topological skyrmion textures in chiral magnets** — •Markus Garst
SYCE 1.5	Mon	17:30–18:00	HSZ 02	**Learning through ferroelectric domain dynamics in solidstate synapses** — Sören Boyn, Gwendal Lecerf, Stéphane Fusil, Sylvain Saïghi, Agnès Barthélémy, Julie Grollier, Vincent Garcia, •Manuel Bibes

Sessions

KR 1.1–1.8	Mon	9:30–12:30	GER 37	**Various Topics I (with DF)**
KR 2.1–2.6	Wed	9:30–11:30	MER 02	**X-Ray Imaging, Holography, Ptychography and Tomography (with MI)**
KR 3.1–3.6	Wed	18:00–20:00	P4	**Crystallography - poster session**

Annual General Meeting of the Crystallography Division

Tue 18:00–19:00 HSZ 204

- Report
- Any other business

KR 1: Various Topics I (with DF)

Nano- and microstructured dielectrics / thin films
Optical and nonlinear optical properties, photonic
High- and low-k-dielectrics
Dielectric surfaces and interfaces

Chair: Martin Diestelhorst

Time: Monday 9:30–12:30 Location: GER 37

KR 1.1 Mon 9:30 GER 37

Octahedral tilt nanostructure in bismuth-based relaxors — •Wolfgang Donner[1], Florian Pforr[1], Marton Major[1], Uwe Stuhr[2], and Bertrand Roessli[2] — [1]Technische Universität Darmstadt, Germany — [2]Paul Scherrer Institut, Switzerland

Among the lead-free ferroelectrics, (1-x)$Na_{1/2}Bi_{1/2}TiO_3$-x $BaTiO_3$ is one of the most promising material systems. The dielectric properties around the morphotropic phase boundary at x = 0.06 are comparable to those of commonly used lead-containing ferroelectrics. However, the atomistic mechanisms leading to the relaxor properties are still unclear.

We performed a diffuse neutron scattering study in order to reveal the nanostructure of the octahedral tilt disorder of the oxygen anions. Our results show the coexistence of multiple tilt systems over a wide temperature range and a strong temperature dependence of the respective domain sizes. On this basis, we propose a model of the nanostructure featuring chemically pinned tetragonal platelets in a rhombohedral matrix. The different tilt domains are separated by a cubic intermediate phase. Furthermore, a strong temperature dependence of the planar defect density was found, which peaks at the depolarization temperature. These features react strongly to the application of an external electric field and their temperature dependence is clearly correlated with the dielectric permittivity.

KR 1.2 Mon 9:50 GER 37

Robust in-plane ferroelectricity over room temperature in atomic-thick SnTe — •Kai Chang[1,2], Junwei Liu[3,2], Haicheng Lin[2], Na Wang[2], Kun Zhao[2], Yong Zhong[2], Xiaopeng Hu[2], Wenhui Duan[2], Liang Fu[3], Qi-Kun Xue[2], Xi Chen[2], Shuai-Hua Ji[2], and Stuart Parkin[1] — [1]NISE, Max-Planck Institute of Microstructure Physics, Weinberg 2, Halle 06120, Germany — [2]State Key Laboratory of Low-Dimensional Quantum Physics, Department of Physics, Tsinghua University, Beijing 100084, China — [3]Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA

Stable ferroelectricity with high transition temperature in nanostructures is needed for miniaturizing ferroelectric devices. Here, applying molecular beam epitaxy (MBE) and variant temperature scanning tunneling microscopy (VT-STM), we have studied the stable in-plane spontaneous polarization in atomic-thick SnTe, down to a 1-unit cell (UC) limit. The ferroelectric transition temperature T_c of 1-UC SnTe film is greatly enhanced from the bulk value of 98 K [1] and reaches as high as 270 K. Moreover, 2- to 4-UC SnTe films show robust ferroelectricity at room temperature [2]. Recent high temperature STM experiments show that the ferroelectricity of 2- and 3-UC SnTe films persists even up to 380 K, comparable with the classical perovskite ferroelectric $BaTiO_3$. [1] M. Iizumi et al., J. Phys. Soc. Jpn. 38, 443 (1975). [2] K. Chang et al., Science, 353, 274 (2016).

KR 1.3 Mon 10:10 GER 37

Flexoelectric impact on the polarization switching dynamics in thin ferroelectric films — •Ivan Vorotiahin[1,2], Anna Morozovska[2], Eugene Eliseev[3], and Yuri Genenko[1] — [1]Institut für Materialwissenschaft, Technische Universität Darmstadt, Jovanka-Bontschits-Str. 2, 64287 Darmstadt, Deutschland — [2]Institute of Physics, National Academy of Sciences of Ukraine, 46, pr. Nauky, 03028 Kyiv, Ukraine — [3]Institute for Problems of Materials Science, National Academy of Sciences of Ukraine, Krjijanovskogo 3, 03142 Kyiv, Ukraine

Flexoelectric effect (or flexocoupling) is one of the properties of solid state materials that couples the gradient of electric polarization with the gradient of mechanical strain. It exists virtually in all solids, but has so small magnitude that it cannot be effectively observed in most of them. However, with the reduction of dielectric film thickness, it might obtain a significant influence on the properties of dielectrics.

A process of domainless polarization switching in the tetragonal ferroelectric $BaTiO_3$ has been modelled, using relations of Landau-Ginzburg mean-field theory. Static distributions of electric polarization and other relevant quantities, including electrostatic potential, donor and electron concentrations, as well as dynamics of polarization switching are obtained and analysed. A role of the flexocoupling is estimated for both statics and dynamics. It appeared, that whilst having a negligible influence on the static distributions, flexocoupling can remarkably affect polarization switching times and the values of critical fields under which the switching occurs.

KR 1.4 Mon 10:30 GER 37

Crystalline high-pressure phases in the Bi–Co system — •Leonore Wiehl[1], Shrikant Bhat[1], Iliya Radulov[1], Konstantin Skokov[1], Michael Dürrschnabel[1], Leopoldo Molina-Luna[1], Sabrina Sicolo[1], Leopold Diop[1], Dmitriy Karpenkov[1], Norimasa Nishiyama[2], Hans-Joachim Kleebe[1], Karsten Albe[1], Ralf Riedel[1], and Oliver Gutfleisch[1] — [1]Fachbereich Material- und Geowissenschaften, Technische Universität Darmstadt, Darmstadt 64287, Germany — [2]DESY, Hamburg 22607, Germany

$RECo_5$ (RE = rare-earth) compounds are known as materials with high magnetocrystalline anisotropy [1]. They crystallize in the $CaCu_5$ structure type, space group $P\frac{6}{m}mm$. On searching for RE-free magnetic materials, which could replace the classical NdFeB magnets, MCo_5 type materials were considered as promising candidates. The existence of crystalline MCo_5 and MFe_5 (M = Bi, Ca, Zr) phases and their magnetic properties were explored. Here we report on the Bi-Co system. Samples with starting compositions 5:1 & 1:1 were subjected to high pressure (15.6 GPa) and temperature (900°C) in a multianvil press at DESY, Hamburg. The recovered products were characterized by X-ray diffraction with synchrotron radiation (ALS, Berkeley), SEM/EDX, and magnetic measurements. They proved to be a mixture of several crystalline phases, with the most prominent phase Bi_3Co [2]. The search for new phases was complemented by DFT calculations.

Financial support by the excellence program LOEWE "RESPONSE" is gratefully acknowledged. [1] K. Strnat et al., J. Appl. Phys. 38 (1967) 1001 [2] S. Tencé et al., J.Phys.: Condens. Matter 26 (2014) 395701

20 min. break

KR 1.5 Mon 11:10 GER 37

Tunability of polymeric whispering gallery mode micro-lasers — •Tobias Siegle[1], S. Schierle[1], S. Krämmer[1], A. M. Flatae[1,2], M. Remmel[1], B. Richter[3], S. Nocentini[2], C. Parmeggiani[2], H. Zeng[2], M. Burresi[2], D. Wiersma[2], S. F. Wondimu[4], P. Schuch[4], C. Koos[4], and H. Kalt[1] — [1]Institute of Applied Physics, KIT, Karlsruhe, Germany — [2]European Laboratory for Non-Linear Spectroscopy, Sesto Fiorentino, FI, Italy — [3]Zoological Institute, KIT — [4]Institute of Microstructure Technology, KIT

Realizing tunable micro-optical devices, e.g., filters or lasers is a challenging task. A possibility is to use mechanically flexible structures. However, often lithographic fabrication and the rigidity of conventional materials induce an inflexibility. Here, we demonstrate that the flexibility of polymers can be utilized for widely tunable photonic circuits.

We review the fabrication of polymeric whispering gallery mode (WGM) micro-lasers and show their superiority in post-fabrication configuration tuning. The first example demonstrates resonance tuning by exploiting liquid crystal elastomers (LCE). When integrated into the cavity, a LCE cylinder can function as a micro-actuator modifying the resonator diameter and hence tuning the WGM resonances.

Polymers allow substrate-independent fabrication based on direct laser writing. As a second example we present the flexible coupling of WGM cavities structured on elastomer substrates. Reducing the inital inter-cavity gap through deformation of the substrate leads to the formation of photonic molecules. Tunable coupling is verified by exponential trends in the intensities of arising super-modes.

KR 1.6 Mon 11:30 GER 37

Interface engineering in all-oxide $Ba_xSr_{1-x}TiO_3$ thin-film varactors with highly conducting $SrMoO_3$ electrodes — •Patrick Salg[1], Aldin Radetinac[1], Dominik Walk[2], Holger Maune[2], Rolf Jacoby[2], Philipp Komissinskiy[1], and Lambert Alff[1] — [1]Institute of Materials Science, TU Darmstadt, Germany — [2]Institute for Microwave Engineering and Photonics, TU Darmstadt, Germany

We present epitaxial varactor heterostructures utilizing highly conducting oxide $SrMoO_3$ bottom electrodes with a room-temperature resistivity of 30 $\mu\Omega$cm [1] grown by pulsed laser deposition using $SrMoO_4$ targets. During thin film synthesis, highly reductive conditions are essential to achieve a Mo^{4+} state in the $SrMoO_3$ thin film. In contrast to the growth conditions of $SrMoO_3$, the growth of $Ba_xSr_{1-x}TiO_3$ films requires a high oxygen partial pressure of 1.5 mTorr. In order to prevent oxidation of the underlying $SrMoO_3$ layers during growth of $Ba_xSr_{1-x}TiO_3$, a $SrTiO_3$ layer was grown between $SrMoO_3$ and $Ba_xSr_{1-x}TiO_3$. The effectivity of this $SrTiO_3$ interlayer as an oxygen diffusion barrier was investigated by X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS). The use of a $SrTiO_3$ interlayer allows a successful epitaxial growth of varactor heterostructures with high electric tunability of up to 80 % and low losses at microwave frequencies.

[1] A. Radetinac *et al.*, *Highly conducting $SrMoO_3$ thin films for microwave applications*, Appl. Phys. Lett. **105**, 114108 (2014).

KR 1.7 Mon 11:50 GER 37

The pyroelectric coefficient of free standing GaN grown by HVPE — •Sven Jachalke[1], Patrick Hofmann[2], Gunnar Leibiger[3], Frank S. Habel[4], Erik Mehner[1], Tilmann Leisegang[1,4], Dirk C. Meyer[1], and Thomas Mikolajick[2,5] — [1]Institute for Experimental Physics, TU Bergakademie Freiberg, Leipziger Str. 23, 09599 Freiberg, Germany — [2]NaMLab gGmbH, Nöthnitzer Str. 64, 01187 Dresden, Germany — [3]Freiberger Compound Materials GmbH, Am-Junger-Löwe-Schacht 5, 09599 Freiberg, Germany — [4]Samara National Research University, Moskovskoye Shosse 34, Samara 443086, Russia — [5]Institute for Semiconductors and Microsystems, TU Dresden, Nöthnitzer Str. 64, 01187 Dresden, Germany

Here, we present the first temperature dependent measurements of the pyroelectric coefficient of free standing, and strain free GaN grown by hydride vapour phase epitaxy (HVPE). The Sharp-Garn method is applied to extract the pyroelectric coefficient from the electrical current response of the crystals subjected to a sinusoidal temperature excitation in a range of 0°C to 160°C. To avoid compensation of the pyroelectric response by an internal conductivity, insulating GaN crystals were used by applying carbon, manganese and iron doping during HVPE growth. Different pyroelectric coefficients observed at room temperature due to the doping correlate well with the change of the lattice parameter c. The obtained data is compared to previously published theoretical and experimental values of thin film GaN and discussed in terms of a strained lattice.

KR 1.8 Mon 12:10 GER 37

Confocal Raman analysis of diffusion profiles in ion exchanged waveguides in PPKTP — •Julian Brockmeier, Michael Rüsing, Christof Eigner, Laura Padberg, Gerhard Berth, Christine Silberhorn, and Artur Zrenner — Department Physik, Universität Paderborn, 33098 Paderborn, Germany

KTP presents a promising material system for integrated quantum optical applications. Integrated quantum optical devices require the fabrication of waveguides, which can be achieved in this material via the ion exchange of Potassium by Rubidium. An optimized fabrication of these structures requires a detailed understanding of the induced changes in the material structure, such as the diffusion profile. Here the confocal Raman imaging technique presents one of the foremost methods for a three dimensional spatial analysis of the material properties. Within this work periodically poled KTP (PPKTP) waveguides have been visualized by Raman imaging. For a more detailed analysis of the induced material changes the data processing has been improved and now allows to map the changes of the FWHM shift and intensity of peaks in the Raman spectra. Based on this optimized method, spectral features have been identified, which are sensitive to the concentration of the ion exchanged Rubidium.

KR 2: X-Ray Imaging, Holography, Ptychography and Tomography (with MI)

Time: Wednesday 9:30–11:30 Location: MER 02

Invited Talk KR 2.1 Wed 9:30 MER 02

X-ray Microscopy: Imaging the Chemistry Inside — •Christian G. Schroer — Photon Science, DESY, Notkestr. 85, 22607 Hamburg — Institut für Nanostruktur- und Festkörperphysik, Universität Hamburg, Jungiusstr. 11, 20355 Hamburg

One key strength of hard X-ray microscopy is that it can image the inner structures of an object without destructive sample preparation. Exploiting various X-ray analytical contrasts, such as fluorescence, diffraction, and absorption, the elemental, structural, and chemical information can be obtained from inside a sample, e. g., a chemical reactor. Conventional X-ray microscopy is currently limited by X-ray optics to a few tens of nanometers. One way to overcome this limitation is scanning coherent X-ray diffraction microscopy also known as ptychography [1]. It can be combined with spectroscopy to obtain chemical information on a given element of interest [2]. In combination with tomography, the three-dimensional structure of an object can be reconstructed with unprecedented spatial resolution [3]. Here, an overview is given over multimodal X-ray imaging for materials research at modern synchrotron radiation sources.

[1] J. Rodenburg, H. Faulkner, Appl. Phys. Lett. 85, 4795 (2004); P. Thibault, et al., Science 321, 379 (2008); A. Schropp, et al., Appl. Phys. Lett. 96, 091102 (2010); A. Schropp, et al., Appl. Phys. Lett. 100, 253112 (2012); J. Reinhardt, et al., Ultramicroscopy 173, 52 (2017).

[2] R. Hoppe, et al., Appl. Phys. Lett. 102, 203104 (2013).

[3] M. Dierolf, et al., Nature 467, 436 (2010); M. Holler, et al., Scientific Reports 4, 3857 (2014).

KR 2.2 Wed 10:00 MER 02

Imaging with hard X-rays and Nanometer Resolution using Multilayer Zone Plates — •Jakob Soltau[1], Christian Eberl[2], Tim Salditt[1], Hans-Ulrich Krebs[2], and Markus Osterhoff[1] — [1]Röntgenphysik, Uni-Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen — [2]Materialphysik, Uni-Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen

The resolution of zone plates is determined by their smallest zone width. Multilayer zone plates (MZP) can be fabricated using the process of pulsed laser deposition, which allows zone width of 5 nm and less and therefore enabling imaging of X-rays on a nanometer scale [1]. The central challenge in the development of hard X-ray nano-focusing MZPs is the fulfilling of the Bragg condition across the zone plate. To achieve this the individual zones need to be tilted. Latest experiments using tilted-MZPs at synchrotron sources demonstrated successfully a resolution of a few nanometer in a wide X-ray energy range from 7 keV at DESY/Petra III and for the first time with photon energies above 100 keV at ESRF. A new setup and a motorized stage significantly reduced the set-up and measuring time in scanning X-ray microscopy allowing high resolution imaging of soft- and hard-matter samples in a shorter time. In addition to the experiments, 3D simulations have been performed. The propagation of electromagnetic waves inside and behind the MZP proved the advantage of circular MZPs to achieve very high photon flux densities in a single focal point. The simulations were revealing interaction processes like e.g. dynamical diffraction inside the MZPs. [1] Eberl, C. et al. Appl. Surf. Sc

KR 2.3 Wed 10:15 MER 02

The Fluence-Resolution Relationship in Holographic and Coherent Diffractive Imaging — •Johannes Hagemann and Tim Salditt — Institut für Röntgenphysik, Friedrich-Hund-Platz 1, University Göttingen, 37077 Göttingen

The simple question "Which resolution do I get for the invested photon fluence?" is extremely important for x-ray imaging of radiation sensitive specimen, such as biological cells and tissues. This work [1] presents a numerical study of the fluence-resolution behavior for two coherent lens-less x-ray imaging techniques. To this end we compare

in numerical experiments the fluence-resolution relationship of inline near-field holography (NFH) and far-field coherent diffractive imaging (CDI). To achieve this, we carry out the phase reconstruction using iterative phase retrieval algorithms on simulated noisy data. Using the incident photon fluence on the specimen as control parameter we study the achievable resolution for two exemplary phantoms (cell and bitmap). A survey based on maximum likelihood estimation [2] of CDI and NFH showed in principle no difference in the encoded information of the measured data for a given fluence. In the current approach we assess the actual reconstructability of the CDI/NFH data via direct phase retrieval. We use then the Fourier Ring Correlation as measure of reconstruction quality i.e. the achievable resolution. Our results indicate a superior performance of holography compared to CDI, for the same fluence and phase reconstruction procedure. [1] J. Hagemann and T. Salditt, Acta Crystallogr. A, (in review) [2] T. Jahn et al., Acta Crystallogr. A, (2017), 73, 1-11

KR 2.4 Wed 10:30 MER 02

Simulations towards high magnification setups in X-ray Talbot-interferometry — •Andreas Wolf, Veronika Ludwig, Jens Rieger, Max Schuster, Maria Seifert, Georg Pelzer, Thilo Michel, Gisela Anton, and Stefan Funk — ECAP - Erlangen Centre for Astroparticle Physics, Universität Erlangen-Nürnberg, Erwin-Rommel-Str. 1, 91058 Erlangen

Compared with the traditional attenuation contrast, X-ray Talbot-interferometry can yield additional information in terms of the differential phase contrast (DPC) and the dark field contrast (DFC) images.

In this imaging modality, which is primarily pursued in the field of medical diagnostics and soft tissue imaging, the Talbot effect leads to the generation of self images of a grating in the beam path. With respect to the thus created spatial reference pattern and by introducing a second grating, the aforementioned contrast modalities can be retrieved either via a phase-stepping approach or by using Moiré-fringes in a single-shot scheme.

In this contribution, we present simulation studies of Talbot-interferometer-based setups featuring high magnifications towards future applications for imaging at XFEL-beamlines and in the field of laboratory astrophysics where a high magnification of object structures is needed to resolve the generated shocks.

15 min. break

KR 2.5 Wed 11:00 MER 02

X-Ray Phase-Contrast Tomography with Anisotropic Source Conditions — •Malte Vassholz, Leon Merten Lohse, and Tim Salditt — Institute for X-Ray Physics, University of Göttingen, Germany

Hard x-ray tomography offers a unique capability to nondestructively map out the three-dimensional structure of a body or material. A major challenge for high-resolution and/or phase-contrast tomography in the laboratory, is the lack of high-brilliance table-top x-ray sources. By suitable generalization of the tomographic measurement geometry and the reconstruction framework, one can significantly relax the brilliance/coherence condition in one of the two lateral source dimensions [1], opening up new opportunities towards nanoscale resolution with low-brilliance table-top x-ray sources. To this end, the framework of the two-dimensional Radon transform, which is the common basis for most analytical x-ray tomography applications, is replaced by the three-dimensional Radon transform. We show applications for absorption tomography as well as phase-contrast tomography for anisotropic source conditions with aspect ratios larger than two orders of magnitude in the lateral source dimensions.

[1] M. Vassholz, B. Koberstein-Schwarz, A. Ruhlandt, M. Krenkel, and T. Salditt, Phys. Rev. Lett. 116, 088101 (2016).

KR 2.6 Wed 11:15 MER 02

Core-shell-shell nanowires studied by coherent x-ray nanobeam — •Arman Davtyan[1], Vincent Favre-Nicolin[2], Ryan B. Lewis[3], Hanno Küpers[3], Lutz Gelhaar[3], Dominik Kriegner[4], Ali Al-Hassan[1], Otmar Loffeld[1], and Ullrich Pietsch[1] — [1]Faculty of Science and Engineering,University of Siegen,57068 Siegen,Germany — [2]The European Synchrotron,71 Avenue des Martyrs,Grenoble,France — [3]Paul-Drude-Institut für Festkörperelektronik,Hausvogteiplatz 5-7,D-10117 Berlin,Germany — [4]4 Department of Condensed Matter Physics,Charles University, Ke Karlovu 5,121 16 Prague 2,Czech Republic

Core-shell-shell heterostructure nanowires (NWs) with 140nm GaAs core, 10nm In(0.10)Ga(0.90)As inner shell and 30nm GaAs outer shell have been investigated by combining coherent x-ray diffraction imaging (CXDI) and ptychograpy in the Bragg geometry. NWs were grown on a prepatterned substrate. Individual nanowires were measured at the ID01 beamline of the ESRF with coherent x-rays of 9keV energy and 150x200 nm full width half maximum (FWHM). 2D ptychography at GaAs (111) Bragg reflection was applied to investigate the nanowire along the growth axis. Ptychographic reconstruction shows the homogeneous structure of the wire along the growth axis. CXDI was applied to record the 3D reciprocal space maps around the symmetric GaAs (111) reflection at different heights along the NW growth axis.

KR 3: Crystallography - poster session

Time: Wednesday 18:00–20:00 Location: P4

KR 3.1 Wed 18:00 P4

Structural and magneto-electric investigations of Erythrosiderites — •Tobias Fröhlich[1], Daniel Brüning[1], Ladislav Bohatý[2], Petra Becker[2], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Kristallographie, Universität zu Köln

Most erythrosiderites of the form $A_2[FeX_5(H_2O)]$ are magneto-electric without multiferroicity. However, in 2013 it was found that the compound $(NH_4)_2[FeCl_5(H_2O)]$ is multiferroic. A comparison of macroscopic and microscopic properties of different compounds of this family reveals interesting insights into the structural order and magnetic coupling. While the crystal structures of most erythrosiderites can be described with space group *Pnma*, $Cs_2[FeCl_5(H_2O)]$ has space group *Cmcm*. In contrast to the other compounds [1, 2], its magnetic structure is not yet directly determined. However, there are investigations of macroscopic quantities, which allow to predict the magnetic structure [3]. We present a neutron study of the magnetic structure of $Cs_2[FeCl_5(H_2O)]$, which perfectly explains these measurements. Furthermore, $Cs_2[FeCl_5(H_2O)]$ exhibits a structural phase transition which was discovered in 1987 [4]. By single crystal X-ray diffraction, we solved the structural distortion associated with this transition, which involves a slight monoclinic distortion into space group $C2/c$.

[1] M. Gabás et al. (1995), J. Phys. Condens. Matter **7** 4725-4738 [2] J. Rodrígues-Velamazán, et al. (2015), arXiv [3] M. Ackermann et al. (2014), J. Phys. Condens. Matter **26** 506002 [4] J. Chadwick et al. (1987), J. Phys. C: Solid State Phys. **20** 3979-3983

KR 3.2 Wed 18:00 P4

Investigation of new phases in the Ba-Si phase diagram under high pressure by ab initio structural search — •Jingming Shi[1], Wenwen Cui[1], José Flores-Livas[2], Alfonso San-Miguel[1], Silvana Botti[3,1], and Miguel Marques[4,1] — [1]Institut Lumière Matière, UMR5306 Université Lyon 1-CNRS, Université de Lyon, F-69622 Villeurbanne Cedex, France — [2]Department of Physics, Universität Basel, Klingelbergstr. 82, 4056 Basel, Switzerland — [3]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [4]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

Barium silicides are versatile materials that have attracted attention for a variety of applications in electronics and optoelectronics. Using an unbiased structural search based on a particle-swarm optimization algorithm combined with density functional theory calculations, we investigate systematically the ground-state phase stability and structural diversity of Ba–Si binaries under high pressure. The phase diagram turns out to be quite intricate, with several compositions stabilizing/destabilizing as a function of pressure. In particular, we identify novel phases of BaSi, $BaSi_2$, $BaSi_3$, and $BaSi_5$ that might be synthesizable experimentally over a wide range of pressures. Our results not only clarify and complete the previously known structural phase diagram, but also provide new insights for understanding the Ba–Si

binary system.

KR 3.3 Wed 18:00 P4

Watching the Verwey transition of Magnetite by Timeresolved X-Ray diffraction — •Alexander von Reppert[1], Jan-Etienne Pudell[1], Flavio Zamponi[1], Azize Koc[2], Stephan Geprägs[3], Jose Emilio Lorenzo[4], Luc Ortega[5], Matthias Reinhardt[2], and Matias Bargheer[1,2] — [1]Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht Str. 24-25, 14476 Potsdam, Germany — [2]Helmholtz-Zentrum Berlin BESSY II, Albert-Einstein Str. 15, 12489 Berlin, Germany — [3]Walther-Meißner-Institut, Bayerische Akademie d. Wissenschaften, 85748 Garching, Germany — [4]Institut Nèel, CNRS & Univ. Grenoble Alpes, 38042 Grenoble, France — [5]Laboratoire de Physique des Solides, CNRS, Univ. Paris-Sud, Université Paris-Saclay, 91405 Orsay, France

We present timeresolved X-Ray diffraction from a 300 nm thin Magnetite(Fe3O4) film that is driven across the Verwey transition by fs-laser excitation. The prototypical insulator to metal transition at 123 K is accompanied by a peak intensity increase and peak width decrease of structural Bragg peaks, which we attribute to the destruction of trimerons that lead to inhomogeneous lattice strain in the low T phase. Our systematic investigations of the lattice dynamics yield two timescales: An ultrafast peak width drop - probably due to electronic processes - which is subsequently enhanced by transport and equilibration of the excitations. Complementary to our lab-based Plasma X-Ray source we conducted measurements at the XPP beamline at the synchrotron BESSY II where we observe that the recovery timescale depends crucially on the proximity to the transition temperature.

KR 3.4 Wed 18:00 P4

Detection of pressure and density waves (acustic waves) in liquid crystal near the phase transition temperature by gold nano particle — •Ricardo Rose, Andre Heber und Frank Cichos — Universität Leipzig Fakultät für Physik und Geowissenschaften, Leipzig, Germany

Recent studies have shown, that the intensity of a polarized laser beam can be modulated by a second heating laser beam, which excites plasmons on gold nanoparticles (AuNp) positioned in liquid crystal (LC). The exited AuNp dissipate the energy as heat into the LC. If the LC is near below the phase transition point from nematic phase to isotropic phase, the dissipated heat will suffice to build an isotropic bubble around the AuNp. The size of the bubble can be controlled by the amount of supplied energy. While the polarization within the nematic phase is rotated due to different refractive indices for the ordinary and extraordinary axis similar to a $\lambda/2$ - plate, the polarization will be conserved within the isotropic phase. If an analyzer is placed behind the LC, the intensity of the probe laser beam can be modulated by the optical path length within the nematic phase and their disturbance within the isotropic bubble around the laser heated AuNp. In this study we investigate, if the deformation of the isotropic bubble by acoustical waves and the linked modulation of the probe laser beam intensity at constant, unmodulated power of the heating laser will be clearly detectable, while the ambient temperature is near the phase transition temperature. If that can be proven, we will able to design a microphone at nano size.

KR 3.5 Wed 18:00 P4

Ga^{3+} Substitution in the Brownmillerite-Type Phase $Ca_2Fe_2O_5$: Structural and Spectroscopic Investigations — •Quirin Stahl[1,2], Andreas Reyer[1], Reinhard Wagner[1], Gerold Tippelt[1], and Günther J. Redhammer[1] — [1]Department Chemistry and Physics of Materials, University of Salzburg, Austria — [2]Institute of Structural Physics, Technische Universität Dresden

Brownmillerite-type compounds with the general formula $A_2B'_{2-x}B_xO_5$, where A = alkaline earth metals and B'/B = group III or transition-metal atoms, are among the most frequently studied oxygen-deficient perovskites. 61 synthetic single-crystal samples of $Ca_2Fe_{2-x}Ga_xO_5$ with $0.00 \leq x \leq 1.328$ have been investigated by single-crystal X-ray diffraction at RT. We find that pure $Ca_2Fe_2O_5$ and samples up to x = 0.989 have space group *Pnma*, Z = 4, whereas samples with x > 0.989 show $I2mb$ symmetry, Z = 4. We also performed a detailed Raman study of Ga^{3+} and Al^{3+} doped $Ca_2Fe_2O_5$. The polarized Raman measurements of $Ca_2Fe_{2-x}Ga_xO_5$ single-crystals enable us to assign eleven of the thirteen theoretically predicted A_g modes. Furthermore the change from *Pnma* to $I2mb$ space group symmetry is reflected by a significant change of two Raman modes below 150 cm^{-1}. These Raman modes are obviously linked to changes of the Ca-O bond lengths at the phase transition. To complete the study of the $Ca_2Fe_{2-x}Ga_xO_5$ series, we have performed a detailed Mössbauer spectroscopic study as a function of the chemical composition, mainly to fix site occupation number by a second, independent method beside XRD.

KR 3.6 Wed 18:00 P4

Synthesis and controlled growth of α-RuCl3 crystals on the nanoscale via chemical vapour transport (CVT) — •Martin Grönke, Mihai-Ionut Sturza, Barbara Eichler, Sandra Schiemenz, Victoria Eckert, Silke Hampel, and Bernd Büchner — IFW Dresden

Crystal growth of different transition metal halogenides representing a very up to date research topic in solid state chemistry surface physics. Among the interest for materials with strong anisotropic bonding-dependent interactions, resulting frustration effects could stabilize new patterns of cooperative magnetic interactions, or even a spin-liquid-state. One candidate to realize a Kitaev spin model is the layered honeycomb magnet α-Rutheniumchloride (α-RuCl3) with strongly frustrated, anisotropic interactions between spin-orbit entangled jeff = 1/2 Ru3+ magnetic moments.

Physical properties in nanoscale systems may differ from the respective bulk phase and could even lead to novel physical properties. Herein we present to our knowledge the first approach to synthesize phase pure α-RuCl3 crystals on the nanoscale via chemical vapour transport (CVT). To understand the growth mechanisms and to optimize the synthesis we performed thermodynamic modelling with the program Tragmin. We obtained very thin single crystals by CVT with heights around 40 nm. The crystal habit is characterized by means of SEM, TEM and AFM. Furthermore EDX, WDX, XRD, micro-RAMAN and SQUID-VSM measurements proving composition, phase-purity and predicted magnetic properties.