Crystalline Solids and their Microstructure Division
Fachverband Kristalline Festkörper und deren Mikrostruktur (KFM)

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Overview of Invited Talks and Sessions

(Lecture rooms EMH 025, EMH 225, E 020, and E 124; Poster E)

Invited Talks

KFM 1.1	Mon	9:30–10:00	EMH 025	**Collective nano-optomechanics and liquids** — •Ivan Favero
KFM 1.2	Mon	10:00–10:30	EMH 025	**Whispering gallery optical parametric oscillators** — •Ingo Breunig
KFM 2.1	Mon	9:30–10:00	EMH 225	**Atomic-resolution imaging of electronic inversion layers at ferroelectric domain walls** — •Julia Mundy, J. Schaab, Y. Kumagai, A. Cano, M. Stengel, I. Kung, D. Gottlob, H. Doganay, M. Holtz, R. Held, Z. Yan, E. Bourret, C. Schneider, D. Schlom, D. Muller, R. Ramesh, N. Spaldin, D. Meier
KFM 2.7	Mon	11:30–12:00	EMH 225	**Understanding the dielectric enhancement from domain walls in conventional and relaxor ferroelectrics** — •Andrew Rappe
KFM 5.1	Mon	15:00–15:30	EMH 025	**Whispering-gallery-like modes in two and three dimensional microcavities** — •Martina Hentschel
KFM 6.1	Mon	15:00–15:30	EMH 225	**First-principles studies of ferroelectric and ferroelastic domain walls** — •Jorge Íñiguez
KFM 6.7	Mon	17:15–17:45	EMH 225	**Probing STO domain walls with scanning SQUID microscopy** — •Beena Kalisky
KFM 10.1	Tue	9:30–10:00	EMH 225	**Insights into the Inside provided by Coherent X-ray Imaging** — •Tim Salditt
KFM 13.1	Wed	9:30–10:00	E 020	**Advanced Cell Adhesion of Modified Ultrananocrystalline Diamond Surfaces** — •Cyril Popov
KFM 13.5	Wed	11:20–11:50	E 020	**CVD diamond for high power electronic devices** — •Verena Zürbig
KFM 14.1	Wed	9:30–10:00	EMH 025	**Resource-efficient dielectric materials for short-time energy storage** — •Stephan Krohns
KFM 14.7	Wed	12:00–12:30	EMH 025	**Dielectric Polymer Nanocomposites for Electrical Energy Storage** — •Qing Wang
KFM 15.1	Wed	9:30–10:00	EMH 225	**Oxygen vacancy controlled functionalities at interfaces of multiferroic tunnel junctions.** — •Jacobo Santamaria
KFM 18.1	Wed	15:00–15:30	E 124	**Application of Diamond Technology to Microwave Systems in Nuclear Fusions Machines** — •Giovanni Grossetti, Gaetano Aiello, Francesco Mazzocchi, Andreas Meier, Sabine Schreck, Peter Spaeh, Dirk Strauss, Theo Scherer
KFM 19.1	Wed	15:00–15:30	EMH 025	**Electrical double layer capacitors, Insights from fundamental research and their impact on storage devices** — •Gudrun Reichenauer
KFM 20.1	Wed	15:00–15:30	EMH 225	**Merging Nonlinear Optics and Multiferroic Heterostructure Design** — •Manfred Fiebig
KFM 23.1	Thu	9:30–10:00	EMH 025	**3D Nanoprinting via Focused Electron Beams** — •Harald Plank, Robert Winkler, Jason Fowlkes, Philip Rack
KFM 23.5	Thu	11:20–11:50	EMH 025	**Diffractive X-ray Optics for Synchrotrons and Free Electron Lasers - a challenge from the lithographer's point of view** — •Christian David

KFM 24.1	Thu	9:30–10:00	E 124	**Discovering Ancient Secrets in Aluminum Alloys – A New Combination of Analytical Techniques and ab-initio Calculations** — •Torsten E.M. Staab, Danny Petschke, Frank Lotter, Elischa Bläss
KFM 26.1	Thu	15:00–15:30	EMH 025	**Electron Beam Lithography and Ion Beam Patterning for Applications in Quantum Technology** — •Jörg Stodolka, Michael Kahl, Axel Rudzinski, Sven Bauerdick

Invited talks of the joint symposium SYVC

See SYVC for the full program of the symposium.

SYVC 1.1	Wed	15:00–15:30	H 0105	**Magneto-ionic control of interfacial magnetism** — •Geoffrey Beach
SYVC 1.2	Wed	15:30–16:00	H 0105	**Ionic Control of Materials Beyond Interfaces** — •Dustin Gilbert
SYVC 1.3	Wed	16:00–16:30	H 0105	**Microscopic Mechanisms of Memristive Switching in Metal Oxides** — •Rainer Waser, Stephan Menzel, Regina Dittmann
SYVC 1.4	Wed	17:00–17:30	H 0105	**In-situ and operando SQUID magnetometry under electrochemical control** — •Roland Würschum, Markus Gössler, Gregor Klinser, Eva-Maria Steyskal, Heinz Krenn
SYVC 1.5	Wed	17:30–18:00	H 0105	**Reversible chemistry as a tool for dynamic control of physical properties** — •Robert Kruk, Subho Dasgupta, Bijoy Das, Horst Hahn

Invited talks of the joint symposium SYAM

See SYAM for the full program of the symposium.

SYAM 1.1	Fri	9:30–10:00	H 0105	**Bringing Dino-Birds to life – Synchrotron X-ray fluorescence and Raman imaging of ancient materials** — •Uwe Bergmann
SYAM 1.2	Fri	10:00–10:30	H 0105	**Linear and Nonlinear Optical Properties of Cultural Heritage Materials** — •Marta Castillejo
SYAM 1.3	Fri	10:30–11:00	H 0105	**Morphology and topology of multiscale pore networks: Imaging structural alteration and hydric invasion** — •Pierre Levitz
SYAM 1.4	Fri	11:15–11:45	H 0105	**Painting cracks: a way to reveal physical properties of matter** — •Ludovic Pauchard
SYAM 1.5	Fri	11:45–12:15	H 0105	**Finite element analysis and biomechanical interpretation of fossil material properties** — •Emily Rayfield

Sessions

KFM 1.1–1.8	Mon	9:30–12:50	EMH 025	**Whispering Gallery Mode Resonators I**
KFM 2.1–2.10	Mon	9:30–12:45	EMH 225	**Ferroelectric Domain Walls I (joint session KFM/TT)**
KFM 3.1–3.10	Mon	9:30–13:10	E 124	**Crystal Structure, Defects, Real Structure and Microstructure in Materials**
KFM 4.1–4.12	Mon	15:00–18:30	EB 301	**Skyrmions I (joint session MA/KFM/TT)**
KFM 5.1–5.8	Mon	15:00–18:10	EMH 025	**Whispering Gallery Mode Resonators II**
KFM 6.1–6.10	Mon	15:00–18:30	EMH 225	**Ferroelectric Domain Walls II (joint session KFM/TT)**
KFM 7.1–7.9	Mon	15:00–18:20	E 124	**Microstructure of thin films / TEM-based Nanoanalysis**
KFM 8.1–8.10	Tue	9:30–12:15	EB 202	**Multiferroics and magnetoelectrics I (joint session MA/KFM)**
KFM 9.1–9.13	Tue	9:30–13:15	EB 301	**Skyrmions II (joint session MA/TT/KFM)**
KFM 10.1–10.11	Tue	9:30–13:40	EMH 225	**Spectroscopy and Microscopy I with X-rays and Ions**
KFM 11.1–11.5	Tue	10:00–11:40	EMH 025	**Dielectric, Elastic and Electromechanical Properties**
KFM 12.1–12.9	Wed	9:30–12:00	EB 202	**Multiferroics and magnetoelectrics II (joint session MA/KFM)**
KFM 13.1–13.8	Wed	9:30–12:50	E 020	**Diamond I**
KFM 14.1–14.7	Wed	9:30–12:30	EMH 025	**Materials for Energy Storage I (joint session KFM/CPP)**
KFM 15.1–15.11	Wed	9:30–12:45	EMH 225	**Multiferroic Oxide Thin Films and Heterostructures I (joint session KFM/TT/MA)**
KFM 16.1–16.9	Wed	9:30–13:00	H 2032	**Lithography I: Focused Electron Beam Induced Processing: 3D Nano-Printing for Material Science (Focussed Session): Morning Session (joint session DS/KFM)**

KFM 17.1–17.14	Wed	15:00–18:30	EB 301	**Skyrmions III (joint session MA/TT/KFM)**
KFM 18.1–18.10	Wed	15:00–17:30	E 124	**Diamond II + Poster**
KFM 19.1–19.7	Wed	15:00–17:50	EMH 025	**Materials for Energy Storage II (joint session KFM/CPP)**
KFM 20.1–20.10	Wed	15:00–18:15	EMH 225	**Multiferroic Oxide Thin Films and Heterostructures II (joint session KFM/TT/MA)**
KFM 21.1–21.11	Wed	15:00–18:00	H 2032	**Lithography II: Focused Electron Beam Induced Processing: 3D Nano-Printing for Material Science (Focussed Session): Afternoon Session (joint session DS/KFM)**
KFM 22	Wed	18:30–19:00	EMH 025	**Annual General Meeting of the KFM division**
KFM 23.1–23.8	Thu	9:30–12:50	EMH 025	**Lithography III: Lithography and Structuring (joint session KFM/DS)**
KFM 24.1–24.7	Thu	9:30–12:20	E 124	**Spectroscopy and Microscopy II with Positrons**
KFM 25.1–25.11	Thu	9:30–13:30	EMH 225	**Ferroics and Multiferroics (joint session KFM/TT/MA)**
KFM 26.1–26.8	Thu	15:00–18:10	EMH 025	**Lithography IV: Lithography and Structuring (joint session KFM/DS)**
KFM 27.1–27.35	Thu	15:00–17:00	Poster E	**Postersession KFM**
KFM 28.1–28.13	Fri	9:30–13:00	H 0110	**Complex Oxides: Bulk Properties, Surfaces and Interfaces (joint session TT/MA/KFM)**

Annual General Meeting of the Crystalline Solids and their Microstructure Division

Mittwoch 18:30–19:00 Raum EMH 025

- Bericht
- Verschiedenes

KFM 1: Whispering Gallery Mode Resonators I

Organizer: Christoph Marquardt - Max Planck Institute for the Science of Light - Erlangen

Time: Monday 9:30–12:50 Location: EMH 025

Invited Talk KFM 1.1 Mon 9:30 EMH 025

Collective nano-optomechanics and liquids — •Ivan Favero — Université Paris Diderot, CNRS, France

We present a new technique to resonantly tune ensembles of nanophotonic/mechanical resonators. The technique builds on the recent experimental development of nano-optomechanics in the liquid-state [1]. Laser light injected into the optical mode of a first resonator immersed in a liquid triggers an etching process, leading to a fine-tuning of the resonators dimensions. The evolution of dimensions is monitored continuously by spectrally tracking the associated optical resonance. This tuning process, dubbed resonant photo-electrochemical etching, is naturally scalable to multiple resonators and has already allowed us to resonantly tune small ensembles (2 to 5 units) [2]. As a first application of this technique, we explore the resonant optical interaction of multiple and distant nano-optomechanical systems. Light flowing unidirectionally along a chain of nano-optomechanical oscillators is observed to produce their frequency-locking above a certain threshold, which represents a first example of collective phenomenon in optomechanics [3]. Our experiments are explained by a minimal semi-classical model, and set the grounds for more advanced quantum experiments.

Acknowledgements: the work presented involved contribution by E. Gil-Santos, W. Hease, A. Lemaitre, M. Labousse, C. Ciuti and G. Leo

[1] Nature Nanotech 10, 810 (2015) [2] Nature Comm 8, 14267 (2017). [3] Phys Rev Lett 118, 063605 (2017).

Invited Talk KFM 1.2 Mon 10:00 EMH 025

Whispering gallery optical parametric oscillators — •Ingo Breunig — Department of Microsystems Engineering - IMTEK, University of Freiburg, Georges-Köhler-Allee 102, 79110 Freiburg, Germany — Fraunhofer Institute for Physical Measurement Techniques IPM, Heidenhofstraße 8, 79110 Freiburg, Germany

Continuous-wave optical parametric oscillators (cw OPOs) combine narrow-linewidth emission with a large wavelength tuning range far beyond that of lasers. Conventionally, these devices are based on a nonlinear-optical crystal surrounded by a mirror cavity.

In whispering gallery optical parametric oscillators (WGR OPOs), light is guided by total internal reflection in a spheroidally-shaped millimeter-sized nonlinear-optical crystal. They provide oscillation thresholds in the (sub)-mW range. However, WGR OPOs are intrinsically triply-resonant. One might assume that wavelength tuning of is much more difficult to control here compared with that of conventional mirror-based singly-resonant systems.

Nevertheless, several experimental studies revealed that the output wavelengths of whispering gallery optical parametric oscillators can be tuned in well-defined steps over hundreds of nanometers by temperature variation and mode-hop-freely to MHz-wide resonances of alkali atoms. WGR OPOs are operated in a spectral range from wavelengths below 600 nm to ones beyond 8000 nm. Thus, these light sources - despite of their intrinsic triple resonance - might serve as compact and wavelength flexible devices for various applications.

KFM 1.3 Mon 10:30 EMH 025

Widely tunable polymer-based photonic devices — Tobias Siegle, •Johann Frank, Stefan Schierle, Michael Remmel, Matthias Migeot, Carolin Klusmann, and Heinz Kalt — Institute of Applied Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

Whispering gallery mode (WGM) resonators have a wide range of applications such as optical sensors, lasers or filters and modulators. Using polymers as resonator material and exploiting the flexibility of elastomeric substrates enables a tunability that further enhances the functionality of photonic devices. In this contribution we demonstrate a fine, reversible and spectrally wide resonance tuning using a novel type of WGM resonators. Further we report on the realization of photonic molecules with tunable coupling. Resonance tuning is achieved using a split-disk geometry - two opposing half-disks structured with direct laser writing onto a elastomeric substrate. Calibrated straining of the substrate allows reversibly tuning the distance between the half-disks and hence the resonance wavelength. Laser emission from dye-doped split-disk resonators reveals a wide tunability of more than three times the free spectral range. Similarly, adjacent goblet-shaped resonators are structured on the elastomer using direct laser writing. Resolving the laser emission spectroscopically and spatially while reducing the coupling gap demonstrates the formation of photonic molecules. Variation of the gap width and hence the coupling strength results in tunable laser-mode intensities, in particular in super-mode formation and mode vanishing due to the Vernier effect.

KFM 1.4 Mon 10:50 EMH 025

Electrical tuning of polymer-based photonic devices on a dielectric polymer substrate — •Matthias Migeot, Tobias Siegle, Michael Remmel, and Heinz Kalt — Institute of Applied Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

Whispering gallery mode (WGM) resonators are versatile photonic structures which have a great variety of applications. A prominent example is given by coupling of two or more WGM resonators to photonic molecules or coupled resonator optical waveguides (CROWs). In this context, it is desirable to dynamically and reversibly tune the coupling strength between multiple resonators as well as the individual resonance wavelengths. In contrast to commonly used semiconductor or silica-based resonators, polymers provide large flexibility to achieve the required tuning capabilities even fabricated in high-precision mass production. In this contribution we use a dielectric polymer as substrate for coupled WGM resonators. The substrate consists of a prestreched PDMS thin-film which is contacted from both sides with polymeric electrodes. If the electrodes are structured appropriately a high DC voltage can be applied to the electrodes which leads to a local relaxation of the substrate and thereby to a reduction of the distances on the substrate. We show first results on the independent control of both, the coupling strength between multiple resonators and the resonance wavelength of an individual (split-disk) resonator.

20 min break

KFM 1.5 Mon 11:30 EMH 025

Mid-infrared whispering gallery optical parametric oscillators — •Yuechen Jia[1], Kevin Hanka[1], Karsten Buse[1,2], and Ingo Breunig[1,2] — [1]Laboratory for Optical Systems, Department of Microsystems Engineering - IMTEK, University of Freiburg, Georges-Köhler-Allee 102, 79110 Freiburg, Germany — [2]Fraunhofer Institute for Physical Measurement Techniques IPM, Heidenhofstraße 8, 79110 Freiburg, Germany

The mid-infrared (mid-IR) spectral window is of great interest because it allows for high-resolution spectroscopy of nearly all gas molecules. Whispering-gallery-resonator (WGR)-based continuous-wave optical parametric oscillators (CW OPOs), which combine high miniaturization and large wavelength tunability, are emerging as efficient frequency-conversion devices for applications in the mid-IR. Based on traditional nonlinear optical materials such as LiNbO3 or KTP, however, CW OPOs are limited to output wavelengths shorter than 5 μm due to the onset of multi-phonon absorption. In this contribution, we report about the fabrication of high-quality-factor whispering gallery resonators made out of AgGaSe2, CdSiP2 and orientation-patterned GaP crystals, which exhibit the highest nonlinear coefficients and broadest infrared transparency ranges among all practical nonlinear optical crystals. With these WGRs, additionally, CW OPOs with low oscillation thresholds and wide tunability in the mid-IR spectral range of 2-8 μm are realized.

KFM 1.6 Mon 11:50 EMH 025

Phase transition studies using second-harmonic phonon spectroscopy — •Christopher J. Winta, Sandy Gewinner, Wieland Schöllkopf, Martin Wolf, and Alexander Paarmann — Fritz-Haber-Institut der MPG

Nonlinear optical spectroscopy constitutes a powerful tool for the investigation of crystalline solids and their structure. Apart from improved sensitivity compared to linear techniques, it offers additional experimental degrees of freedom which can be used to selectively study different symmetry components of the detected signal. The mid-infrared (MIR) spectral region is particularly interesting as it contains optical

phonon resonances which themselves carry symmetry information.

Here, we demonstrate MIR second-harmonic (SH) phonon spectroscopy [1] as a symmetry-sensitive technique to investigate structural phase transitions, using the $\alpha \rightarrow \beta$ transition of quartz as a case example. A MIR free-electron laser grants access to essentially all optical phonon resonances of quartz which are selectively investigated with regard to their temperature-dependent behavior upon T_c. The data show a critical phase transition behavior of the phonon frequencies, damping rates and SH peak amplitudes. Additionally, certain phonon modes become IR-forbidden in the higher symmetry β-phase and consequently disappear from the SH spectra upon the phase transition.

Given its sensitivity to crystal structure and symmetry, our novel technique presents itself as a promising tool for the study of structural phase transitions in polar dielectrics, e.g. ferroelectrics or multiferroics.

[1] Winta et al., arXiv:1710.02097 (2017)

KFM 1.7 Mon 12:10 EMH 025

Single photon generation in a whispering gallery mode resonator — •Golnoush Shafiee[1,2], Gerhard Schunk[1,2], Florian Sedlmeir[1,2], Alexander Otterpohl[1,2], Ulrich Vogl[1,2], Dmitry Strekalov[1,2], Harald G. L. Schwefel[3], Gerd Leuchs[1,2], and Christoph Marquardt[1,2] — [1]MPL, Erlangen, Germany — [2]FAU, Erlangen, Germany — [3]University of Otago, Dunedin, New Zealand

Single photons are an important resource for quantum information processing since they are reliable long distance carriers for quantum information. The generation of high quality single photons with controllable narrow spectral bandwidths and central frequencies is key to facilitate efficient coupling of any atomic system to non-classical light fields. Here, we report on a fully tunable, narrow band and efficient source of non-classical light, in particular single photons [1,2], based on a crystalline whispering gallery mode resonator. It is made of lithium niobate and works based on spontaneous parametric down-conversion where a pump photon decays due to material nonlinearties into two single cavity modes of different wavelengths. The central wavelength of the emitted light can be tuned over hundreds of nanometers [3].

Currently, we are working on generating polarization entangled photon states with our compact and monolithic source, which opens up novel possibilities for creating the central building block for proposed quantum repeater schemes.

[1] M. Förtsch et al., Nat. Commun. 4, 1818 (2013). [2] J. U. Fürst et al., Phys. Rev. Lett. 106, 113901(2011). [3] G. Schunk et al., Optica 2, 773-778 (2015).

KFM 1.8 Mon 12:30 EMH 025

Generation of non-classical light in a nonlinear crystalline whispering gallery mode resonator — •Alexander Otterpohl[1,2], Florian Sedlmeir[1,2], Thomas Dirmeier[1,2], Ulrich Vogl[1,2], Gerhard Schunk[1,2], Golnoush Shafiee[1,2], Dmitry Strekalov[1,2], Harald G. L. Schwefel[3], Tobias Gehring[4], Ulrik L. Andersen[4], Gerd Leuchs[1,2], and Christoph Marquardt[1,2] — [1]Max Planck Institute for the Science of Light, Staudtstr. 2, 91058 Erlangen, Germany — [2]Institute of Optics, Information and Photonics, University Erlangen-Nürnberg, Staudtstr. 7 B2, 91058 Erlangen, Germany — [3]The Dodd-Walls Centre for Photonic and Quantum Technologies, Department of Physics, University of Otago, 730 Cumberland Street, 9016 Dunedin, New Zealand — [4]Department of Physics, Technical University of Denmark, Fysikvej, 2800 Kgs. Lyngby, Denmark

Macroscopic crystalline whispering gallery mode resonators (WGMR) made out of $LiNbO_3$ are a versatile source of non-classical light generated via optical parametric down-conversion [1]. This is a process where one photon is split into two photons called signal and idler. Both photons are correlated due to energy conservation, which affects the statistical fluctuations in certain measurements. We report how non-classical light can be efficiently generated and present the prospects of possible applications within the field of optomechanics [2].

[1] J. U. Fürst et al., Phys. Rev. Lett. **106**, 113901 (2011).
[2] V. Peano et al., Phys. Rev. Lett. **115**, 243603(2015).

KFM 2: Ferroelectric Domain Walls I (joint session KFM/TT)

Organizer: Sergey Artyukhin - Istituto Italiano di Tecnologia - Genova (Italy)

Time: Monday 9:30–12:45 Location: EMH 225

Invited Talk KFM 2.1 Mon 9:30 EMH 225

Atomic-resolution imaging of electronic inversion layers at ferroelectric domain walls — •Julia Mundy[1], J. Schaab[2], Y. Kumagai[2], A. Cano[3], M. Stengel[4,5], I. Kung[6], D. Gottlob[7], H. Doganay[7], M. Holtz[8], R. Held[8], Z. Yan[2,9], E. Bourret[9], C. Schneider[7], D. Schlom[8], D. Muller[8], R. Ramesh[9,10], N. Spaldin[2], and D. Meier[2,11] — [1]Harvard University — [2]ETH Zurich — [3]Université de Bordeaux, ICMCB — [4]ICREA Institució Catalana de Recerca i Estudis Avançat — [5]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB — [6]TU Berlin — [7]Forschungszentrum Julich — [8]Cornell University — [9]Lawrence Berkeley National Laboratory — [10]UC Berkeley — [11]Norwegian University of Science and Technology

Ferroelectric domain walls hold great promise as functional two-dimensional materials because of their unusual electronic properties. Particularly intriguing are the so-called charged walls where a polarity mismatch causes local, diverging electrostatic potentials requiring charge compensation and hence a change in the electronic structure. These walls can exhibit significantly enhanced conductivity and serve as a circuit path. Here we use atomic-resolution STEM-EELS to directly probe the charge transfer at these charged ferroelectric domain walls in $ErMnO_3$. Our direct quantification of the charge transfer to the domain boundary gives insight into the the formation and eventual activation of an inversion layer that acts as the channel for the charge transport. The findings provide new insight into the domain-wall physics in ferroelectrics.

KFM 2.2 Mon 10:00 EMH 225

Charged domain walls and point defect-DW interactions in hexagonal manganites — Didrik Rene Småbråten[1], Quitin Meier[2], Sandra Helen Skjaervoe[1], Thomas Tybell[1], Dennis Meier[1], and •Sverre Magnus Selbach[1] — [1]NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]Materials Theory, ETH Zurich, Zürich, Switzerland

Charged head-to-head and tail-to-tail ferroelectric domain walls (DW) in hexagonal manganites are stable because of the improper nature of the ferroelectricity in these materials, and it has been experimentally shown that their electronic properties can differ strongly from bulk. First principles studies of charged DWs are scarce and the inherent electrostatic fields make DFT calculations challenging. Here we combine density functional theory (DFT) calculations with a continuum model based on Landau theory to study the properties of charged DWs in $YMnO_3$, $InMnO_3$ and isostructural $YGaO_3$. We find excellent agreement between the micro- and macroscopic models, and show that the Mexican hat energy landscape of hexagonal maganites derived from Landau theory also emerges naturally from DFT calculations of their DWs. Head-to-head and tail-to-tail DW are structurally inequivalent due to the different local chemical bonding. We formulate a general criterion based on polarization and band gap for when charged DWs become conducting. Finally, we study interactions between DWs and oxygen interstitials and vacancies by DFT.

KFM 2.3 Mon 10:15 EMH 225

Local control of chemical structure in a functional oxide — •Donald M. Evans[1], Theodor S. Holstad[1], Aleksander B. Mosberg[2], Per-Erik Vullum[2], Didrik Småbråten[1], Sverre Selbach[1], Antonius T. J. Van Helvoort[2], and Dennis Meier[1] — [1]Department of Materials Science and Engineering, NTNU, Norway — [2]Department of Physics, NTNU, Norway

Since the suggestion to use ferroelectric domain walls (DWs) in nanoelectronics, there has been a great deal of research into their properties. The most obvious use of DWs with enhanced conductivity was as nano-wires. But more recently, research is moving towards using the DW as the functional element within a circuit, e.g. as a switch or diode. This approach could allow whole circuit elements to be replaced by a single sub nanometre wide object - an option with clear

technological potential. Attractive as this concept is, the research is still in its embryonic stage with many unanswered questions, not least, how to connect these DW circuit elements. In this work, we demonstrate how an atomic force microscope (AFM) can be used to change the functional properties locally: that is, we can use an AFM to write conducting strips on demand with all the position and control associated with AFM techniques. This is demonstrated on a hexagonal manganite ($ErMnO_3$) and foreshadows the possibility to interconnect functional DWs into nanoscale circuits. To better understand this ability to locally control functional properties, these modified regions were analysed with both TEM, and EELS.

KFM 2.4 Mon 10:30 EMH 225

Anomalous domain wall motion in Cu-Cl boracite: negative permittivity in an improper ferroelectric? — •Charlotte Cochard[1], Joseph G.M. Guy[1], Michael P. Campbell[1], Roger W. Whatmore[2], Amit Kumar[1], Raymond G.P. McQuaid[1], and Marty Gregg[1] — [1]Queen's University Belfast, Belfast UK — [2]Imperial College London, London, UK

Negative capacitance has attracted a lot of attention recently thanks to its potential to enable shorter switching time of transistors. It has been observed in systems as diverse as p-n junction, electrochemical systems, and ferroelectrics. To date, no single-phase material has been reported to exhibit negative capacitance.

In this work, we show that regions in a boracite crystal ($Cu_3B_7O_{13}Cl$) exhibit anomalous electric-field-induced movement of charged domain walls, consistent with negative permittivity. Boracites naturally display domain wall configurations, seen to be electrically active by current mapping [1]. While applying an electric field across some of these charged walls, we observed that domains with polarisation components pointing opposite to the electric field grow at the expense of domains with polarisation components aligned with the field. Thus dP/dE is negative and hence permittivity is negative. This behaviour is proposed to originate from the improper ferroelectric nature of the boracite: the elastic energy payoff, due to polarisation-strain coupling, is greater than the work done in generating increased polarisation against the applied electric field.

[1] R.G.P. McQuaid, et al. Nat. Commun. 8, 15105 (2017).

15 min break

KFM 2.5 Mon 11:00 EMH 225

Interplay between point defects and domain wall mobility in improper ferroelectric $YMnO_3$ — •Didrik René Småbråten, Dennis Meier, and Sverre Magnus Selbach — Norwegian University of Science and Technology (NTNU), Trondheim, Norway

Understanding the domain wall (DW) dynamics in ferroelectrics is key to controlling and fine-tune the domain structure and hence the ferroelectric properties. The DW dynamics strongly couple to the defect chemistry in the material, where stationary dopants may act as pinning centers or mobile defects may move with the DWs. The overall aim of this study is to give chemical guidelines for how to control the domain wall mobility via defect chemistry. Improper ferroelectric $YMnO_3$ has a complex and exotic DW structure, including neutral, as well as positively and negatively charged DWs. Furthermore, the material has a large chemical flexibility being robust against donor and acceptor doping of its cation sublattices, and it is stable under both oxygen deficiency and excess. This unique flexibility makes $YMnO_3$ an ideal model system for studying the interplay between DW mobility and defect chemistry. From density functional theory (DFT) calculations we show how changes in the two cation sublattices affect the DW mobility. In addition, we study how mobile anion defects couple to the DW movement and determine if they move with or pin the DWs.

KFM 2.6 Mon 11:15 EMH 225

Conducting domain wall networks in $TbMnO_3$ and $BiFeO_3$ — •Mart Salverda[1], Wilson Acevedo[2], Diego Rubi[2], Saeedeh Farokhipoor[1], and Beatriz Noheda[1] — [1]Zernike Institute for Advanced Materials, Groningen, The Netherlands — [2]CNEA and INN, Buenos Aires, Argentina

Ferroelastic domain walls in thin films of some complex oxides show a higher conductivity than the domains [1][2]. This effect is proposed to originate from the accumulation of ionic species at the domain walls due to the presence of strain gradients [2][3][4]. In a recent study [5] we propose a model that accounts for the electrical behavior measured in $TbMnO_3$ thin films using macroscopic techniques, by assuming that the structural domain walls that are present in these films [6] are conducting. From the model, the value of the sheet resistance of the domain walls has been extracted. To further investigate the validity of this approach for other materials, we perform a similar analysis on systems incorporating thin films of $BiFeO_3$ where the domain walls are already proven to be conducting. Our aim is to elucidate the intrinsic transport properties of the domain walls.

[1] J. Seidel et al., *Nature Materials* **8**, 229 (2009) [2] S. Farokhipoor and B. Noheda, *Physical Review Letters* **107**, 127604 (2011) [3] E. Salje and H. Zhang, *Phase Transitions* **82**, 452 (2009) [4] T. Rojac et al., *Nature Materials* **16**, 322 (2017) [5] W. Román et al. (in preparation) [6] S. Farokhipoor et al., *Nature* **515**, 379 (2014)

Invited Talk KFM 2.7 Mon 11:30 EMH 225

Understanding the dielectric enhancement from domain walls in conventional and relaxor ferroelectrics — •Andrew Rappe — University of Pennsylvania, Philadelphia, PA, USA

The dielectric properties of ferroelectric materials are a key driver of smart materials applications. In this talk, two key aspects of anomalous dielectric enhancement will be analyzed: domain walls and relaxor ferroelectrics. A comprehensive theoretical viewpoint will be sketched that unifies these aspects, based on multi-scale materials modeling.

Incorporating quenched Coulombic disorder in ferroelectrics disrupts and changes the character of this transition; instead of a sharp transition in a small temperature range, these oxide alloys exhibit "relaxed" transitions over 100-200 K and are called "relaxor ferroelectrics." I will describe how a first-principles based multi-scale model can reveal the dynamic and statically correlated motions of ions that lead to relaxor behavior, and I will discuss their promise for next-generation piezoelectric and dielectric material systems, with emphasis on the emergent stabilization of a high density of low-angle domain walls.

I will also present molecular dynamics simulations of 90 degree domain walls (separating domains with orthogonal polarization directions) in the ferroelectric material $PbTiO_3$ to provide microscopic insights that enable the construction of a simple, universal, nucleation-and-growth-based analytical model that quantifies the dynamics of many types of domain walls in various ferroelectrics. This new model illuminates domain wall influence on the dielectric responses of conventional and relaxor ferroelectrics.

KFM 2.8 Mon 12:00 EMH 225

In-situ 4D observation of ferroelectric domain wall dynamics using second-harmonic generation microscopy — •Lukas Wehmeier, Alexander Haussmann, and Lukas M. Eng — Institute of Applied Physics, Technische Universität Dresden, 01062 Dresden, Germany

Second-harmonic generation microscopy (SHGM) allows for the three-dimensional (3D) observation of ferroelectric domain walls (DWs) across millimeter-thick bulk materials [1,2]. For example, this is of supreme value for exploring inclined and charged domain walls [1,3]. Here, we apply SHGM in order to quantify the DW dynamics in triglycine sulfate (TGS) single crystals upon the ferroelectric-to-paraelectric phase transition at the Curie temperature of $\approx 49\,^{\circ}C$ [4]. In addition, we study DW dynamics that are induced by external electric fields.

We show for TGS that SHGM allows exploring such electric-field-induced and temperature-driven DW dynamics in 4D, i.e. in real-time and full 3D imaging.

[1] T. Kämpfe et al., Phys. Rev. B 89, 035314 (2014).
[2] T. Kämpfe et al., Appl. Phys. Lett. 107, 152905 (2015).
[3] C. Godau et al., ACS Nano 11, 4816 (2017).
[4] L. Wehmeier et al., Phys. Stat. Solidi RRL 11, 1700267 (2017).

KFM 2.9 Mon 12:15 EMH 225

Electrical half-wave rectification at improper ferroelectric domain walls — •J. Schaab[1], S. H. Skjaervo[2], S. Krohns[3], X. Dai[1], M. Holtz[4], M. Lilienblum[1], D. A. Muller[4,5], M. Fiebig[1], S. M. Selbach[2], and D. Meier[1,2] — [1]ETH Zürich — [2]NTNU Trondheim — [3]University of Augsburg — [4]Cornell University — [5]Kavli Institute at Cornell for Nanoscale Science

Ferroelectric domain walls represent multifunctional 2D-elements that offer great potential for novel device paradigms. Improper ferroelectrics display particularly promising domain walls, which due to their unique robustness, are the ideal template for imposing the desired electronic behavior. Chemical doping, for instance, induces p- or n-type characteristics and electric fields reversibly switch between

resistive and conductive domain-wall states.

Here, we demonstrate conversion of alternating current (AC) into direct current (DC) output based on neutral 180° domain walls in improper ferroelectric $ErMnO_3$. By combining scanning probe and dielectric spectroscopy, we show that the AC-to-DC conversion occurs for frequencies at which the domain walls are pegged to their equilibrium position. The practical frequency regime and magnitude of the output is controlled by the conductivity of the surrounding domains. Using density functional theory, we attribute the distinct transport behavior to oxygen defects that accumulate at the neutral walls. Our study reveals domain walls acting as 2D half-wave rectifiers, extending domain-wall-based nanoelectronics applications into the realm of AC-technology.

KFM 2.10 Mon 12:30 EMH 225

Unexpected $BiFeO_3$ 71 degree domain wall vibration — •Peng Chen and Sergey Artyukhin — Quantum Materials Theory, Istituto Italiano di Tecnologia, Genova (Italy)

Emergent phenomena excitations at domain walls are attracting enormous attention recently. Recent scanning impedance microscopy (SIM) measurements reveal AC conductance attributed to domain wall-localized phonons, that give important contributions to low-frequency dynamics in ferroic materials. In $BiFeO_3$ the polarization change across 71 degree domain walls is perpendicular to the electric field applied by the SIM tip, and therefore the DW-localized phonon should not be excited by the tip. However, the experimental observations show a violation of this intuitive picture. Here we use Landau-Ginzburg theory and first-principles calculations to address this puzzling behavior.

KFM 3: Crystal Structure, Defects, Real Structure and Microstructure in Materials

Chair: Enrico Langer - Technische Universität Dresden

Time: Monday 9:30–13:10 Location: E 124

KFM 3.1 Mon 9:30 E 124

Higher-Order Topological Insulators — •Frank Schindler[1], Ashley Cook[1], Maia Vergniory[2], Zhijun Wang[3], Stuart Parkin[4], Andrei Bernevig[3], and Titus Neupert[1] — [1]University of Zurich, Switzerland — [2]University of the Basque Country, Spain — [3]Princeton University, USA — [4]Max Planck Institute of Microstructure Physics, Germany

Three-dimensional topological (crystalline) insulators are materials with an insulating bulk, but conducting surface states which are topologically protected by time-reversal (or spatial) symmetries.

Here, we extend the notion of three-dimensional topological insulators to systems that host no gapless surface states, but exhibit topologically protected gapless hinge states. Their topological character is protected by spatio-temporal symmetries, of which we present two cases: (1) Chiral higher-order topological insulators protected by the combination of time-reversal and a four-fold rotation symmetry. Their hinge states are chiral modes and the bulk topology is Z2-classified. (2) Helical higher-order topological insulators protected by time-reversal and mirror symmetries. Their hinge states come in Kramers pairs and the bulk topology is Z-classified.

We provide the topological invariants for both cases. Furthermore, we discuss current developments concerning material realizations of these novel phases of matter.

KFM 3.2 Mon 9:50 E 124

Stability of carbon clathrates: a theoretical investigation — •Conrad Steigemann and Miguel Marques — Martin-Luther-Universität Halle- Wittenberg

Due to their structure, clathrates naturally offer a good possibility to be doped by a variety of atoms to change the properties of the scaffold element drastically. Besides germanium and silicon showing clathrate structures, no stable clathrates of carbon could be found yet. Studies [Zeng et al. 2015] suggest a substitution of single carbon atoms with boron to stabilise the structure.

In this contribution, we perform extensive calculations of the energy landscape of carbon clathrates in order to understand if these can indeed be synthesized. This will be done by using a combination of high-throughput density-functional theory and global structural prediction methods.

KFM 3.3 Mon 10:10 E 124

Band gap engineered multicomponent equitatomic rare earth oxides synthesized by nebulized spray pyrolysis — •Leonardo Velasco Estrada[1], Abhishek Sarkar[1,2], and Horst Hahn[1,2,3] — [1]1Institute of Nanotechnology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — [2]Joint Research Laboratory Nanomaterials, Technische Universität Darmstadt and Karlsruhe Institute of Technology, Alarich-Weiss-Str. 2, 64287 Darmstadt, Germany — [3]Helmholtz Institute Ulm, Electrochemical Energy Storage, Helmholtzstr. 11, 89081 Ulm, Germany

Several multicomponent equitatomic rare earth oxides (ME-REOs) systems containing up to 7 elements (Ce, Gd, La, Nd, Pr, Sm and Y) were synthesized by nebulized spray pyrolysis. The systems showed narrow direct and indirect band gaps in the range of 1.95 * 2.14 eV, respectively. X-ray diffraction as well as transmission electron microscopy confirmed that all the systems crystallized as phase pure fluorite type (fm3m) structure. X-ray photoelectron spectroscopy revealed that Ce and Pr are in a 4+ and in a mixed oxidation state (3+/4+), respectively, while the other constituent elements are in a 3+ oxidation state. In this study the observed narrow band gap is closely related to the presence of multivalent Pr, since the phase pure fluorite type systems that were synthesized without Pr exhibited a band gap $>$ 3eV. Interestingly, the narrow band gaps were not highly affected by the high chemical complexity of the systems. Therefore, this category of materials offers flexibility for band gap engineering and tunability.

KFM 3.4 Mon 10:30 E 124

Zinc-blende and wurtzite phase formation in indium phosphide nanowires grown by template-assisted selective epitaxy — •Philipp Staudinger[1], Stephan Wirths[1], Marta D. Rossell[1,2], Marilyne Sousa[1], Kirsten E. Moselund[1], and Heinz Schmid[1] — [1]IBM Research Zuerich, 8803 Rueschlikon, Switzerland — [2]Electron Microscopy Center, EMPA, 8600 Duebendorf, Switzerland

Group III-V semiconductor nanowires (NWs) are expected to provide a platform for a wide range of future applications such as high-performance field effect transistors and optoelectronic devices. Nanostructures offer a new type of band structure engineering based on the formation of zinc-blende (ZB) - wurtzite (WZ) polytypism. These crystal phases are distinctively different in terms of physical properties facilitating applications such as direct bandgap materials in the 495-570 nm wavelength regime. However, the crystallographic quality of NWs remains difficult to control, resulting typically in the formation of a high number of planar defects. So far, using Template-Assisted Selective Epitaxy (TASE), the growth of WZ phase has not been observed.

We demonstrate that both WZ and ZB crystal phases can be obtained using TASE. InP NWs were selectively grown using metal organic vapor phase epitaxy at temperatures of 625 °C and a V/III ratio of 50 inside predefined hollow oxide templates of varying dimensions. The crystal phase was determined by micro photoluminescence spectroscopy along with scanning transmission electron microscopy. Both ZB and WZ phases were found in nearly pure form, giving promise for novel device applications such as high efficient green LEDs.

KFM 3.5 Mon 10:50 E 124

Local properties of PPKTP waveguide structures probed by Raman spectroscopy — •Julian Brockmeier[1], Michael Rüsing[1], Christof Eigner[1], Laura Padberg[1], Peter Mackwitz[1], Christine Silberhorn[1,2], 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

Periodically poled waveguides in Potassium Titanyl Phosphate (PPKTP) have promising capabilities for integrated quantum optical applications [1]. However a fundamental understanding of the underlying

physics for a defined domain patterning of waveguides, especially in the submicron region, is important. In this context we report on our systematic analysis of periodically poled Rb-exchanged waveguides in KTP in the framework of various fabrication-parameters e.g. melt-composition, exchange-temperature and fabrication order performed by confocal Raman spectroscopy. The vibrational properties of the periodically poled waveguides were determined for different scattering geometries in three dimensions. We found specific phonon modes linked to the stoichiometric/crystallographic structure and to the induced stress.

[1] Marco Fiorentino et al., 'Spontaneous parametric down-conversion in periodically poled KTP waveguides and bulk crystals', OPTICS EXPRESS, 15 (12) 7479 (2007)

20 min. break

KFM 3.6 Mon 11:30 E 124

Phase identification in spark plasma sintered (SPS) Fe-Al-Si powders — •Jaromír Kopeček[1], Jarmila Remiášová[1], Ladislav Klimša[1], Petr Haušild[2], Miroslav Karlík[2], František Laufek[3], Kateřina Nová[4], Jakub Šesták[4], Boris Severa[4], Filip Průša[4], and Pavel Novák[4] — [1]Department of Functional Materials, Institute of Physics of the CAS, Prague, Czech Republic. — [2]Department of Materials, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Czech Republic. — [3]Czech Geological Survey, Prague, Czech Republic. — [4]Department of Metals and Corrosion Engineering, University of Chemistry and Technology Prague, Prague, Czech Republic.

Fe-Al-Si alloys are interesting materials with promising corrosion properties. The components of such alloys are cheap, nevertheless the way of preparation is complicated and increasing the price of the product. Our group investigated properties of Fe - 20 wt. % Al - 20 wt. % Si alloy prepared by mechanical alloying followed by spark plasma sintering under various conditions. The element powders were used for mechanical alloying. The microstructure and phase composition were investigated with optical and electron microscopies (including EDS and EBSD) and X-ray diffraction. It was found that mechanically alloyed powders contain mainly of-stoichiometric binary phases, whereas sintered samples contain significant amount of ternary phase. The phase description is complicated as the phases dimensions are small and composition is off-stoichiometric both in powders or compacted alloys.

KFM 3.7 Mon 11:50 E 124

Size Calibration of IR-Laser Scattering Tomography by using Tailored Oxygen Precipitates in Cz-Si — •Robert Kretschmer[1,3], Andreas Sattler[1], Dawid Kot[2], Gudrun Kissinger[2], and Martin Stutzmann[3] — [1]Siltronic AG, Johannes-Hess-Strasse 24, 84489 Burghausen — [2]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder) — [3]Walter Schottky Institut, Am Coulombwall 3, 85748 Garching

Infrared Light Scattering Tomography (LST) is the standard method for detection of bulk micro defects in silicon. It is mainly used to determine the density of oxygen precipitates, which can act as internal getter for metal impurities during device manufacturing process. Since gettering efficiency depends on precipitate dimensions, bulk defect size is an important parameter to be measured.

We propose to use a size calibration for LST method based on reference wafers with bulk defects of well-defined size, shape and density. These defects have been fabricated through thermal growth of oxygen precipitates. A simulation applying a diffusion-limited model was performed to optimize thermal cycles for reaching pre-defined target defect sizes. The comparison of LST results with TEM shows that precipitate size can be controlled in the relevant calibration range from 20-100 nanometers.

KFM 3.8 Mon 12:10 E 124

Coarsening and growth of metastable γ'' precipitates in Ni-based superalloys — •Felix Schleifer, Markus Holzinger, Yueh-Yu Lin, Michael Fleck, and Uwe Glatzel — Metals and Alloys, University of Bayreuth, Germany

We develop a phase field model for the simulation of diffusion-limited precipitation in Ni-based superalloys with industry-relevant chemical complexity. In the wrought alloy Inconel 718 superior performance at high temperatures is achieved by coherent γ'' precipitations in the fcc matrix. Under non-equilibrium conditions the metastable Ni_3Nb intermetallic compound γ'' with tetragonal structure is the main strengthening phase in the alloy. During heat treatment and aging the formation and coarsening of such precipitates is controlled by Nb-diffusion in the matrix.

The thermodynamic formulation of the model will be validated by comparison to respective CALPHAD equilibrium calculations using the commercial software ThermoCalc. Furthermore, an elastic term is included in the model to account for external loads, anisotropic lattice mismatch stresses as well as elastic inhomogeneities between the considered phases.

This project was recently started as part of the second phase of the DFG priority program 1713. We aim to study steady state growth and coarsening of the precipitated particles as a function of the basic two heat treatment parameters i. e. temperature and time. Phase field studies concerning multiple particles and microstructure evolution under mechanical loading will be carried out subsequently.

KFM 3.9 Mon 12:30 E 124

On the microstructure of the shape memory alloy Co-Ni-Al using complementary diffraction techniques — •Leonid Potapov[1], Enrico Langer[1,2], Katerina Krátká[1], Jaromir Kopeček[3], and Siegfried Däbritz[1] — [1]TU Dresden, IFMP, Dresden, Germany — [2]TU Dresden, IHM, Dresden, Germany — [3]Institute of Physics of the CAS, Prague, Czech Republic

Shape memory alloys can have a quite complex microstructure, making the investigation of their properties very challenging. This work deals with the characterization of austenitic samples of $Co_{38}Ni_{33}Al_{29}$, grown by the Bridgeman method at different pulling rates. In this alloy, a mixture of ordered bcc crystal β matrix and a secondary dendritic fcc γ phase enriched with Co was observed by the combination of X-ray Kossel microdiffraction, EBSD and EDX methods. Thereby the Kossel technique reveals the presence of anisotropic superstructure reflections of the {100} type in the β phase. EBSD linescans into heavily strained β matrix areas suggest a superposition of diffraction patterns of bcc and fcc even at great distances from the phase boundaries. This makes the evaluation of patterns very intricate and may cause problems for automated EBSD. Furthermore, the fcc pattern appears to dominate deeply inside the matrix. This might be caused by Co-rich γ-like micro/nano precipitates, embedded in the matrix and inducing internal strains. In analogy to our previous Kossel measurements, pairs of parallel Kikuchi bands from both patterns can be used to retrieve the orientation relationship between β matrix and γ precipitates, which appears to be close to the Nishiyama-Wasserman relationship.

KFM 3.10 Mon 12:50 E 124

In-situ imaging techniques for the study of magnetocaloric materials — •Anja Waske, Alexander Funk, and Rudolf Schäfer — IFW Dresden

In-situ temperature-dependent magneto-optical imaging is applied to study the thermal hysteresis of magnetocaloric MnFePSi spherical powder-packed beds across their magneto-elastic transition. Cooling and heating imaging series are used to analyze the transition of such a complex powder ensemble. The magnetization versus temperature behavior reconstructed from these local measurements shows very good agreement with integral measurements of the magnetization of the whole packed bed. Hence, local magneto-optical imaging measurements represent the ensemble behavior well if the number of measurements is large enough.

KFM 4: Skyrmions I (joint session MA/KFM/TT)

Time: Monday 15:00–18:30 Location: EB 301

Topical Talk KFM 4.1 Mon 15:00 EB 301

Structure, Energetics, and Deterministic Writing of Skyrmions in Thin Film Ferromagnets — •Felix Büttner — MIT, Cambridge, MA, USA

Room temperature skyrmions were recently observed in magnetic multilayer systems [1-4], most of them in materials with sizable Dyzaloshinskii-Moriya interaction (DMI). In this talk, I will present a unified theory that analytically describes the energy of such skyrmions, including stray fields [1]. We can now rigorously define two types of skyrmions, "stray field skyrmions" and "DMI skyrmions". DMI skyrmions can be sub-10 nm at zero field and room temperature and moved with velocities exceeding 1000 m/s at 10^{12} A/m^2.

Experimentally, I will show that skyrmions can be nucleated by spin-orbit torque current pulses without any applied fields [2]. The nucleation mechanism is robust, ultra-fast (sub-nanosecond), and extremely easy to implement. I will discuss the mechanism of the skyrmion generation and explain why DMI can replace the need for in-plane fields.

[1] Büttner et al., Nat Phys. 11, 225 (2015). [2] Woo et al., Nat Mater. 15, 501 (2016). [3] Moreau-Luchaire et al., Nat Nano. 11, 444 (2016). [4] Boulle et al., Nat Nano. 11, 449 (2016). [5] Büttner et al., arXiv:1704.08489 [6] Büttner et al., Nat Nano. 12, 1040 (2017).

KFM 4.2 Mon 15:30 EB 301

Skyrmion bubble size and density control in Ta/CoFeB/MgO wedges — •Christian Denker[1], Sören Nielsen[2], Enno Lage[2], Jeffrey McCord[2], and Markus Münzenberg[1] — [1]Institut für Physik, Universität Greifswald, Germany — [2]Nanoscale Magnetic Materials - Magnetic Domains, Institute for Materials Science, Universität Kiel, Germany

After the observation of skyrmion bubbles at room temperature in Ta/CoFeB/TaO_x layers by A. Hoffmann's group, skyrmions have been found in various heavy metal/ferromagnet/oxide systems. For skyrmion generation and detection by magnetic tunnel junctions (MTJ), the Ta/CoFeB/MgO system is appealing due to high TMR ratios and its technological maturity. As a starting point typical MTJ bottom electrodes and barriers (5 nm Ta/x CoFeB/3 nm MgO) trilayers with an optional Ru capping were deposited by e-beam evaporation (MgO, Ru) and magnetron sputtering (Ta, CoFeB). We will present our results on skyrmion bubbles observed by magneto-optical Kerr effect microscopy as function of continuous variation of CoFeB thickness. The in- to out-of-plane transition for the magnetic anisotropy is found at about $x = 1.4$ nm. At slightly thinner CoFeB thicknesses skyrmions can be nucleated. Their size can be as small as 300 nm. The influence of CoFeB composition and annealing temperature on the skyrmion formation, as well as skyrmion stability will be discussed.

KFM 4.3 Mon 15:45 EB 301

Small angle neutron scattering experiments of skyrmions far from equilibrium — •Alfonso Chacon[1], Marco Halder[1], Andreas Bauer[1], Wolfgang Simeth[1], André Heinemann[2], Sebastian Mühlbauer[2], and Christian Pfleiderer[1] — [1]Physik Department, Technische Universität München, Germany — [2]Heinz Maier-Leibnitz Zentrum, Garching, Germany

The prospect of the application of magnetic skyrmions in next-generation spintronic devices has recently created substantial scientific interest in this type of magnetic order. Stabilized by thermal fluctuations closed to the paramagnetic order, skyrmion lattices in cubic chiral magnets are constrained to a small window a few Kelvin wide. Recent developments have demonstrated how to expand this regime down to low temperatures by means of supercooling, electrical fields, or uniaxial pressure. Thus, it is possible to study this topological type of magnetism far from equilibrium. We report detailed small angle neutron scattering experiments on skyrmion lattices in B20 compounds at very low temperatures stabilized through fast cooling and discuss the role of disorder and magnetocrystalline anisotropies in their stabilization.

KFM 4.4 Mon 16:00 EB 301

Entropy limited topological protection of skyrmions in $Fe_{1-x}Co_xSi$ — Johannes Wild[1], •Thomas Meier[1], Simon Pöllath[1], Matthias Kronseder[1], Andreas Bauer[2], Alfonso Chacon[2], Marco Halder[2], Marco Schowalter[3], Andreas Rosenauer[3], Josef Zweck[1], Jan Müller[4], Achim Rosch[4], Christian Pfleiderer[2], and Christian Back[1] — [1]Institut für experimentelle und angewandte Physik, Universität Regensburg — [2]Physik-Department, Technische Universität München — [3]Institut für Festkörperphysik, Universität Bremen — [4]Institut für Theoretische Physik, Universität zu Köln

Topologically protected magnetic textures in materials with broken inversion symmetry are considered as future high-density data storage media. The life time of these textures therefore plays a crucial role for data retention. We have used Lorentz transmission electron microscopy to infer the energetics of the topological decay of magnetic skyrmions far from equilibrium in the chiral magnet $Fe_{1-x}Co_xSi$. We investigated the decay of a lattice of sykrmions at different magnetic fields and temperatures by imaging the magnetic configuration of the system in real-time with a high speed camera. We observed that the skyrmion life time τ extracted from these movies depends exponentially on temperature following an Arrhenius law, $\tau \propto \tau_0 \exp(\Delta E/k_B T)$. The prefactor τ_0 of this Arrhenius law changes by more than 30 orders of magnitude for small changes of magnetic field reflecting a substantial reduction of the life time of skyrmions by entropic effects and thus an extreme case of enthalpy-entropy compensation.

KFM 4.5 Mon 16:15 EB 301

Magnetotransport and Hall effect of MnSi thin film under pressure — •David Schroeter[1], Stefan Süllow[1], Dirk Menzel[1], Hiroyuki Hidaka[2], Hideto Okuyama[2], and Hiroshi Amitsuka[2] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [2]Graduate School of Science, Hokkaido University Sapporo, Japan

In the recent years thin films of the B20 compound MnSi became subject of great interest, since the magnetic properties of bulk MnSi are modified due to the dimensional reduction and the uniaxial anisotropy with a suspected stabilized skyrmionic phase [1]. In comparison to bulk material MnSi thin film shows an enhanced ordering parameter with ongoing research about the nature of the magnetic order in thin film state [2].

The ordering temperature and critical fields of MnSi decrease with applied hydrostatic pressure, with thin film material recovering bulk values for the transition temperature at $p_{recover} \approx 2.3$ GPa and a qualitatively similar behavior to bulk MnSi with respect to the ordering temperature above $p_{recover}$ [3]. We present magnetotransport and Hall effect measurements on MnSi thin films under applied pressure of up to around 4 GPa and discuss our results concerning the magnetic phase diagram under pressure.

[1] A. B. Butenko et al., Phys. Rev. B 82, 052403 (2010).
[2] M. N. Wilson et al., Phys. Rev. B 86, 144420 (2012).
[3] J. Engelke et al., Phys. Rev. B 89, 144413 (2014).

KFM 4.6 Mon 16:30 EB 301

Magnetic anisotropy in the itinerant helimagnet MnSi — •Schorsch M. Sauther[1], Andreas Bauer[1], Dirk Grundler[2], Christian Pfleiderer[1], and Marc A. Wilde[1] — [1]Phys.-Dep. E51, TU München — [2]LMGN, IMX, STI, EPF Lausanne

We report torque magnetometry in Manganese silicide (MnSi). In our experiment, we employ cantilever magnetometry in a 2D magnetic field $\vec{B} = B \cdot (\sin\varphi \quad \cos\varphi)$ to measure the torque τ resulting from the anisotropic magnetization $\vec{M}_\perp$ of a high-quality, single-crystalline bulk sample of MnSi. The angular dependence $\tau(\varphi)$ displays distinct oscillations with differently pronounced extrema. The oscillation amplitude between several extrema does not saturate for our maximum field of 4.5 T. In the field dependence $\tau(B)$ we observe an unexpected hysteresis above H_{c2}. Furthermore, the hysteretic behavior below H_{c2} changes drastically with temperature below T_c. We utilize our observations to determine the anisotropy constants and discuss our results in the context of complementary experiments[1].

[1] A. Bauer *et al.*, Phys. Rev. B **95**, 024429 (2017)

15 min break

KFM 4.7 Mon 17:00 EB 301

Inelastic neutron scattering studies of magnons in the field polarized, conical and Skyrmion phase of MnSi — •Lukas Beddrich[1], Tobias Weber[3], Robert Georgii[1,2], and

Peter Böni[1] — [1]Physik-Department E21, Technische Universität München, 85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85748 Garching, Germany — [3]Institut Laue-Langevin (ILL), 38000 Grenoble, France

Cubic chiral magnets, such as MnSi, are prototypical systems for the investigation of various spin structures. They are stabilized by the Dzyaloshinsky-Moriya interaction (DMI), which also gives rise to a universal magnon dispersion [1], [2].

Recently, the effect of non-reciprocal spin wave excitations, which generally emerge from the lack of inversion symmetry, were intensively studied in the field-polarized and helimagnetic phase of MnSi with inelastic neutron scattering [3]. Due to the excellent compatibility between the low-energy theory and the comprehensive measurements, we currently apply a related approach to describe the magnetic excitations found in the skyrmion phase.

[1] M. Janoschek et al. *Phys. Rev. B*, 81:214436, Jun 2010 doi:10.1103/PhysRevB.81.214436

[2] M. Kugler et al. *Phys. Rev. Lett.*, 115:097203, Aug 2015. doi:10.1103/PhysRevLett.115.097203

[3] T. Weber et al. *submitted for publication*

KFM 4.8 Mon 17:15 EB 301

Orientation dependence of the magnetic phase diagram of the chiral magnet Cu_2OSeO_3 — •Marco Halder[1], Alfonso Chacon[1], Andreas Bauer[1], Helmuth Berger[2], and Christian Pfleiderer[1] — [1]Technische Universität München, Physik-Department E21, D-85748 Garching, Germany — [2]École Polytechnique Fédérale de Lausanne, Crystal Growth Facility, CH-1015 Lausanne, Switzerland

In recent years, the cubic chiral insulator Cu_2OSeO_3 attracted great scientific interest, combing the skyrmion lattice phase with strong magneto-electric coupling. We report a comprehensive study of the magnetic properties of single-crystal Cu_2OSeO_3 by means of measurements of the magnetization, ac susceptibility, and specific heat, in particular tracking the influence of crystal orientation, cooling history and demagnetizing effects on the formation of skyrmion order.

KFM 4.9 Mon 17:30 EB 301

Time resolved Lorentz-TEM measurements of dynamical skyrmion lattice defects in Cu_2OSeO_3 — •Simon Pöllath[1], Johannes Wild[1], Lukas Heinen[2], Thomas Meier[1], Matthias Kronseder[1], Leonard Tutsch[1], Andreas Bauer[3], Helmuth Berger[4], Christian Pfleiderer[3], Josef Zweck[1], Achim Rosch[2], and Christian Back[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Deutschland — [2]Institut für Theoretische Physik, Universität zu Köln, Deutschland — [3]Physik-Department, Technische Universität München, Deutschland — [4]Crystal Growth Facility, École Polytechnique Fédérale de Lausanne, Schweiz

We report non-stroboscopic time resolved Lorentz-Transmission-Electron-Microscopy (LTEM) measurements of skyrmion lattice defects in the chiral magnet Cu_2OSeO_3. The multiferroic insulator hosts a hexagonal skyrmion lattice which can be observed in real space using LTEM. It is known, that the radial temperature profile caused by the illumination of the sample with the TEM electron beam sets the skyrmion lattice into rotation [1]. We utilize this effect to study the dynamics of defects and grain boundaries that naturally occur during the lattice rotation. The structural and dynamical behaviour of the defects is similar to that of 2D hexagonal particle lattices and therefore the particle character of the skyrmion in its lattice phase is stressed by our findings [2].

[1] Mochizuki, M. et al. Nat. mater. 13.3 (2014): 241-246

[2] Pöllath S, et al. PRL 118.20 (2017): 207205

KFM 4.10 Mon 17:45 EB 301

Large-scale *ab initio* investigations of complex magnetic textures — •Marcel Bornemann, Sergii Grytsiuk, Paul F. Baumeister, Phivos Mavropoulos, Nikolai S. Kiselev, Samir Lounis, Rudolf Zeller, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We have developed a unique electronic structure code, KKR*nano* [1], specifically designed for petaFLOP computing. Our method scales linearly with the number of atoms, so that we can realize system sizes of up to half a million atoms in a unit cell. Recently, we implemented a relativistic generalization of the algorithm enabling the calculation of complex non-collinear magnetic structures in real space.
We present two applications: (i) In the helimagnet B20-MnGe different experimental groups have observed either a spin spiral in [001] direction or a 3Q-state composed of three spin spirals [2,3]. We present an *ab initio* comparison of both states. (ii) We performed a large-scale evaluation of low-lying thermal excitations, so-called "nodons", in Cr which could explain the formation of a spin density wave in this system [4].
Simulations were performed with computing resources granted by JARA-HPC, Forschungszentrum Jülich and HLRS in Stuttgart.
[1] A. Thiess *et al.*, Phys. Rev. B **85**, 235103 (2012).
[2] O.L. Makarova *et al.*, Phys. Rev. B **85**, 205205 (2012).
[3] T. Tanigaki *et al.*, Nano Lett. **15**, 5438 (2015).
[4] V. Vanhoof *et al.*, Phys. Rev. B **80**, 184420 (2009).

KFM 4.11 Mon 18:00 EB 301

Giant structural response of Dzyaloshinskii-Moriya interaction in MnGe B20 compounds — •Sergii Grytsiuk, Marcel Bornemann, Markus Hoffmann, Bernd Zimmermann, Phivos Mavropoulos, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Non-centrosymmetric cubic B20 materials are currently under intensive investigation. An important feature of these materials is the competition between the antisymmetric Dzyaloshinskii-Moriya interaction (DMI) and the symmetric exchange interaction resulting in a rich variety of magnetic phases with respect to temperature, magnetic fields, material compositions and geometries. The possibility of engineering chiral structures and the effective switching between different magnetic phases requires the investigation of possible factors that influence the strength of the magnetic interactions. In this work, we show by first-principles calculations based on DFT that under pressure magnetic and structural properties of MnGe reveal a hysteretic behavior near the state where energies of high and low spin states coincide. We observe that pressure strongly enhances the DMI (by a factor 5), while the spin-stiffness gets smaller. In order to understand such giant enhancement of the micromagnetic DMI we computed atomistic DMI vectors. Surprisingly, the absolute value of the DMI vectors do not depend significantly on the lattice parameter and the enhancement of micromagnetic DMI stems mainly from the change of the DMI vectors' orientation with respect to bonds between Mn atoms.

KFM 4.12 Mon 18:15 EB 301

Spin-orbit coupling effects in magnetic and response properties of B20 $A_{1-x}B_xGe$ alloys (A, B = Mn, Fe, Co, Rh) — •Sergiy Mankovsky[1], Sebastian Wimmer[1], Svitlana Polesya[1], Nicolas Martin[2], Isabelle Mirebeau[2], and Hubert Ebert[1] — [1]Dept. Chemistry, LMU Munich, D-81377 Munich, Germany — [2]Lab. Léon Brillouin, CEA, CNRS, Uni. Paris-Saclay, France

The composition-dependence of the isotropic exchange (J_{ij}) and Dzyaloshinskii-Moriya interaction (DMI) ($\vec{D}_{ij}$) of $Mn_{1-x}Fe_xGe$, $Mn_{1-x}Rh_xGe$, $Mn_{1-x}Co_xGe$ and $Fe_{1-x}Co_xGe$ B20 alloys have been investigated by first-principles calculations using the relativistic multiple scattering Korringa-Kohn-Rostoker (KKR) formalism. The $D^{\alpha\alpha}$ ($\alpha = x, y, z$) elements of the DMI tensor exhibit a strong dependence on the composition, changing sign at $x \approx 0.85$ in $Mn_{1-x}Fe_xGe$ and at $x \approx 0.5$ in $Fe_{1-x}Co_xGe$, in line with previous theoretical calculations as well as with experimental results. The spin-orbit torque (SOT), anomalous and spin Hall conductivities (AHC and SHC, respectively) of $Mn_{1-x}Fe_xGe$ alloys have been investigated. A sign change at $x \approx 0.5$ is predicted for the Fermi sea contribution to the SOT, as this is closely related to the DMI. In the case of anomalous and spin Hall effects it is shown that the calculated Fermi sea contributions are rather small and the composition-dependence of these effects are determined mainly by the electronic states at the Fermi level. The spin-orbit-induced scattering mechanisms responsible for both effects are suggested to cause the minimum of the AHC and the sign change of the SHC.

KFM 5: Whispering Gallery Mode Resonators II

Organizer: Christoph Marquardt - Max Planck Institute for the Science of Light - Erlangen

Time: Monday 15:00–18:10 Location: EMH 025

Invited Talk KFM 5.1 Mon 15:00 EMH 025

Whispering-gallery-like modes in two and three dimensional microcavities — •Martina Hentschel — Technische Universität Ilmenau, Institut für Physik, Weimarer Str. 25, 98693 Ilmenau

Optical microcavities and microlasers have gained a lot of interest as fascinating model systems for fundamental research and because of their high potential in nanophotonic applications. Their properties are often determined by the resonances of the cavity, i.e., its geometry. The focus of this talk will be on whispering-gallery (WG) type resonances, their dependence on the dimensionality of the system, the role of geometric phases, and the resulting far-field characteristics and application potential, e.g., in sensors.

WG-like resonances form in rotational invariant and even in non-invariant systems such as the so-called Limaçon shape. Their properties depend also on the dimensionality of the system as does the resulting emission characteristics, thereby opening new possibilities of their use in, e.g., sensing applications [1]. We also show that WG-like modes can be strongly influenced in the presence of geometric (Berry, Pancharatnam) phases, for example in the Möbius strip cavity, and how the geometric phase and polarization properties can be controlled by the cavity shape.

[1] J. Kreismann, S. Sinzinger, and M. Hentschel, Phys. Rev. A 95, 011801(R) (2017).

KFM 5.2 Mon 15:30 EMH 025

Hybrid photonic-plasmonic whispering-gallery-mode resonators — •Carolin Klusmann[1], Jens Oppermann[2], Patrick Forster[1], Carsten Rockstuhl[2], and Heinz Kalt[1] — [1]Insitute of Applied Physics, KIT, Karlsruhe, Germany — [2]Institute of Theoretical Solid State Physics, KIT, Karlsruhe, Germany

Hybrid photonic-plasmonic systems combining high-Q dielectric whispering-gallery-mode (WGM) resonators with plasmonic elements are a promising platform to study cQED-phenomena or nonlinear effects. In this contribution, we investigate the modal characteristics of a wedge-like polymeric WGM resonator coated with a thin silver layer which is evanescently coupled to a tapered fiber. The hybrid system is carefully engineered to support three distinct categories of eigenmodes: photonic modes, surface-plasmon-polariton modes, localized at the metal-dielectric interface, as well as hybrid modes. Owing to similar Q-values for both photonic and hybrid modes, and owing to the high sensitivity of the resonance wavelengths to tiny variations in the resonator geometry and permittivity, an assignment of the experimentally observed resonances with the simulated eigenmodes is challenging. Hence, an experimental ansatz is required to identify the measured resonances. FEM simulations considering the interaction with the input waveguide suggest, that measuring the coupling strength of the eigenmodes as a function of the relative horizontal distance between fiber and resonator edge in combination with a polarization dependent excitation allows for an unambiguous classification of the modes. We verify this experimentally.

KFM 5.3 Mon 15:50 EMH 025

High-Q Integrated lithium niobate thin film Whispering Gallery Resonators for Frequency Conversion — •Richard Wolf[1], Ingo Breunig[1,2], and Karsten Buse[1,2] — [1]Department of Microsystems Engineering - IMTEK, University of Freiburg, 79110 Freiburg, Germany — [2]Fraunhofer Institute for Physical Measurement Techniques, 79110 Freiburg, Germany

For realizing non-linear optical frequency converters, lithium niobate whispering-gallery-resonators (WGRs) are most promising due to their high field enhancement by small mode volumes and high Q-factors. Thus, with bulk-WGRs in millimeter size, e.g. optical parametrical oscillation with μW-threshold and conversion efficiencies could be demonstrated. However, WGRs are still rare in commercial products due to the serial and thus expensive fabrication like diamond-blade-cutting with subsequent mechanical polishing. Therefore, integrating WGRs on chip by parallel MEMS fabrication techniques becomes a substantive topic. Compared to bulk WGRs also a 1000 times smaller mode volume can be achieved, especially by using lithium niobate thin film substrates ridge-waveguide WGRs with high refractive index contrast and thus strong light confinement. We report on integrated WGRs based on lithium niobate thin films, made by parallel and thus scalable MEMS fabrication techniques. By using a coupling scheme with tunable coupling efficiency we could couple more than 95 % of pump light into our resonators and achieved intrinsic Q-factors higher than 10^6. We studied non-linear optical effects like second harmonic generation, sum frequency generation and stimulated Raman scattering.

KFM 5.4 Mon 16:10 EMH 025

Self-pumped three-wave mixing in laser-active whispering-gallery resonators — •Simon J. Herr[1], Karsten Buse[1,2], and Ingo Breunig[1,2] — [1]Department of Microsystems Engineering - IMTEK, University of Freiburg, 79110 Freiburg, Germany — [2]Fraunhofer Institute for Physical Measurement Techniques IPM, 79110 Freiburg, Germany

High-Q whispering-gallery resonators (WGRs) made from lithium niobate (LN) have proven to be an excellent platform for highly efficient three-wave mixing. Typically, frequency conversion is induced by pumping whispering-gallery modes (WGMs) of the resonator by means of an external narrow-linewidth light source. Due to the high field enhancement within the high-Q cavity, light-matter interaction is strongly enhanced. Here, we present an important step towards further integration, by using the high-Q cavity not only for nonlinear optics but also for the generation of narrow-linewidth laser light, which is required for pumping nonlinear optical processes. This is achieved by implementing laser-active ions into the host material of the WGR. Importantly, the laser active ions can be excited with cheap light sources, while lasing in high-Q WGMs leads to an intrinsically mode-matched and narrow-linewidth laser oscillation, capable of pumping nonlinear optical processes within the very same high-Q cavity. With these highly integrated devices, self-frequency doubling is achieved in neodymium-doped lithium niobate. A radially poled quasi-phasematching structure allows for self-optical parametric oscillation.

20 min break

KFM 5.5 Mon 16:50 EMH 025

Near infrared cathodoluminescence measurements on paraboloidal and conical silicon photonic nanoresonators — •Sebastian W. Schmitt, Klaus Schwarzburg, and Catherine Dubourdieu — Helmholtz-Zentrum Berlin für Materialien und Energie

Due to the indirect band-to-band transition, spontaneous emission rates in silicon (Si) are low and efficient Si-based solid state lighting remains challenging. The confinement of spectrally matched optical modes can amplify spontaneous emission rates of electronic transitions in Si nanophotonic resonators. Hereby, the amplification is proportional to Q/V, where Q is the quality factor and V is the volume of the resonant mode. This so-called Purcell effect could successfully be applied to improve the performance of Si-based light emitters. Here, Si acts as active or passive resonator material amplifying intrinsic band-to-band or defect transitions or the transitions of added gain media. We show cathodoluminecence (CL) measurements performed in a scanning electron microscope on two novel types of Si photonic resonators with inverted conical and inverted paraboloidal geometry. CL scanning of the resonators by the electron beam at different heights shows a selective excitation of optical whispering gallery modes in the near-infrared wavelength range. A discussion of the excited modes with respect to Q-factor, polarization, relative intensity and resonator geometry shows that the nanoresonators permit a strong and tunable light amplification in the telecom window and accordingly are suitable building blocks for small on-chip solid state lighting devices.

KFM 5.6 Mon 17:10 EMH 025

Whispering Gallery Modes in Self-Assembled Microspheres of Highly Fluorescent Polymers — Daniel Braam[1], Guenther Prinz[1], Kenichi Tabata[2], Soh Kushida[2], Daichi Okada[2], Yohei Yamamoto[2], and •Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University Duisburg-Essen, Germany — [2]Faculty of Pure

and Applied Sciences, University of Tsukuba, Japan

We report on the realization of spherical microresonators by self-assembly of π-conjugated copolymers. These polymers combine the features of being a dye as well as a dielectric. They also enable facile, large-scale fabrication of microspheres with excellent optical and structural properties [1]. Single microspheres were investigated by photoluminescence in the visible regime. The spectra exhibit sharp whispering gallery modes (WGMs) with Q-factors up to 10 000 [2], superimposed upon a broad luminescence background. The high Q-factors, together with the properties of the polymer spheres, make it possible to study the evolution of WGMs, both inside a single sphere, as well as between optically coupled multi-sphere arrangements [3]. Strong optical excitation leads to a slight oblate deformation of the resonators. This results in a splitting of the WGMs, as the high degeneracy of perfectly spherical confinement is lifted [2]. Using suitable polymer blends with tunable fluorescence properties, efficient, long-range unidirectional photon energy transfer ("photon one-way street") can be demonstrated [3].

[1] K. Tabata *et al.*, Sci. Rep. **4**, 5902 (2014).
[2] D. Braam *et al.*, Sci. Rep. **6**, 19635 (2016).
[3] S. Kushida *et al.*, ACS Nano **10**, 5543 (2016).

KFM 5.7 Mon 17:30 EMH 025

WGM resonator technique for condensed matter characterization — Hanna Hlukhova[1], Nataliia Naumova[1], Alexander Barannik[2], Alexey Gubin[2], Irina Protsenko[2], Nikolay Cherpak[2], and •Svetlana Vitusevich[1] — [1]Bioelectronics (ICS-8), Forschungszentrum Juelich, 52425 Juelich, Germany — [2]Usikov Institute for Radiophysics and Electronics, 61085 Kharkiv, Ukraine

WGM resonators represent a key technique in enabling material studies due to their high-quality resonant mode operation using evanescent electromagnetic fields. A very small perturbation introduced by a material under test results in a shift of resonant frequency and change in quality factor, thus reflecting the unique dielectric properties of the material. In this work, we present several developed resonators made of sapphire or quartz materials and discuss the advantages of fabricated measurement cells. WGM resonators of various geometries and materials were suggested in order to utilize the full potential of electromagnetic fields as a test wave interacting with materials, such as single-crystal Fe-pnictides and bioliquids. The resonators were studied using numerical modeling methods. Experimentally obtained quality factors are in good agreement with modeled values. It was also shown that the resonator enables the measurement of the complex permittivity of materials with an error of about 1 %. Microfluid channels combined with WGM resonators operated in the Ka band open up the possibility of contactless measurements for small volumes of biological liquids. This work is supported by DFG project: VI 456/3-1. N.N. greatly appreciates support from the Heinrich Hertz-Foundation.

KFM 5.8 Mon 17:50 EMH 025

Towards a whispering gallery mode resonator based wavemeter — •Thomas Halbauer[1,2], Golnoush Shafiee[1,2], Gerhard Schunk[1,2], Alexander Otterpohl[1,2], Florian Sedlmeir[1,2], Dmitry Strekalov[1,2], Harald G. L. Schwefel[3], Gerd Leuchs[1,2], and Christoph Marquardt[1,2] — [1]Max Planck Institute for the Science of Light, Staudtstr. 2, 91058 Erlangen, Germany — [2]Institute of Optics, Information and Photonics, University Erlangen-Nürnberg, Staudtstr. 7 B2, 91058 Erlangen, Germany — [3]The Dodd-Walls Centre for Photonic and Quantum Technologies, Department of Physics, University of Otago, 730 Cumberland Street, 9016 Dunedin, New Zealand

Macroscopic crystalline whispering gallery mode resonators (WGMR) can provide the possibility for a whispering gallery type wavemeter (WGTW) in just one monolithic device. The frequency spacings between different resonance frequencies of the WGMR represent a unique fingerprint of the frequency of the exciting laser. We use an electro-optic frequency tuning mechanism to shift the fingerprint of an unknown source with fixed frequency. The accuracy is only limited by the linewidth of resonances. In combination with our experimental resonance frequency analysis [1], this unambiguously reveals the excitation wavelength. For achieving the required temperature stability, we implement a scheme based on the differential shift between differently polarized resonance frequencies of an additional locking laser.

[1] G. Schunk *et al.*, Opt. Express **22**, 30795 (2014).

KFM 6: Ferroelectric Domain Walls II (joint session KFM/TT)

Organizer: Sergey Artyukhin - Istituto Italiano di Tecnologia - Genova (Italy)

Time: Monday 15:00–18:30 Location: EMH 225

Invited Talk KFM 6.1 Mon 15:00 EMH 225

First-principles studies of ferroelectric and ferroelastic domain walls — •Jorge Íñiguez — Materials Research and Technology Department, Luxembourg Institute of Science and Technology, Avenue des Hauts-Fourneaux 5, L-4362 Esch/Alzette, Luxembourg

I will present our latest theoretical predictions on how to control the properties of functional oxides, and even induce completely new behaviors, by appropriately engineering their nano-structure, domains or domain walls. I will focus on two different research directions. On one hand, I will discuss ways to engineer ferroelectric and ferroelastic domain walls so they acquire specific properties (conductive, magnetic, topological) not present in the surrounding domains. On the other hand, I will show predictions that ferroelectric domain walls can be used to control heat currents, and can even act as phonon filters. Finally, I will also describe briefly the first-principles-based (second-principles) large-scale simulation methods that we use in most of our investigations.

Works done in collaboration with many colleagues, in particular H.J. Zhao, M.A.P. Gonçalves and C. Escorihuela-Sayalero (LIST); M. Royo, J.A. Seijas-Bellido and R. Rurali (ICAMB-CSIC); and J. Junquera and P. García-Fernández (U. Cantabria). Work at LIST funded by the Luxembourg National Reserach Fund through the CORE (Grant C15/MS/10458889 NEWALLS), PEARL (Grant P12/4853155/Kreisel COFERMAT) and AFR (Grant No. 9934186) programs.

KFM 6.2 Mon 15:30 EMH 225

First-principles prediction of electric skyrmions — •Mauro Gonçalves[1,2], Carlos Escorihuela-Sayalero[1], Pablo García-Fernández[2], Javier Junquera[2], and Jorge Íñiguez[1] — [1]Luxembourg Institute of Science and Technology, Belvaux, Luxembourg — [2]Universidad de Cantabria, Santander, Spain

Nowadays, nontrivial topological spin structures like skyrmions are a focus of interest, as they open the door to novel nano-technologies with huge potential impact. Some authors have discussed electric skyrmions, whereby an exotic arrangement of electric dipoles would yield skyrmion-like structures in ferroelectric materials. Indeed, the recent experimental discovery of a dipole vortices in $PbTiO_3/SrTiO_3$ superlattices [1] has added to earlier theoretical predictions of skyrmions in ferroelectric nano-composites [2], and the possibility of stabilizing electric skyrmions currently attracting a lot of attention.

Following these ideas, we have used first-principles model potentials and large-scale lattice-dynamical simulations [3] to investigate the behavior of ferroelectric nano-domains immersed in a big domain of opposite polarization. Our simulations yield the first prediction of an electric skyrmion in a single phase material. We have also found that these dipole structures can be controlled applying an epitaxial strain or external electric fields, which may open the door to interesting physics and applications.

[1] Damodaran, A. R. et al., Nature Materials **16**, 1003 EP (2017).
[2] Nahas, Y. et al., Nature Communications **6**, 8542 EP (2015).
[3] J.C. Wojdeł, et al., J. Phys.:Condens. Matter **25**, 305401 (2013).

KFM 6.3 Mon 15:45 EMH 225

The impact of domains on phase transitions and the electrocaloric effect - an ab initio based study of $BaTiO_3$. — •Anna Grünebohm[1], Madhura Marathe[2], and Claude Ederer[3] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]Institut de Ciència de Materials de Barcelona, Spain — [3]Materials Theory, ETH Zürich, Switzerland

The electrocaloric effect (ECE) is the adiabatic temperature change induced by a varying external electrical field [1]. Although large temperature changes arise at field-induced first order phase transitions, this re-

sponse may be irreversible due to thermal hysteresis [1-3]. We present an *ab initio* based study of the impact the domain structure makes on such transitions, their thermal hysteresis, and the (reversible) caloric response. As example, we focus on the tetragonal and orthorhombic phases of $BaTiO_3$ [4].

[1] X. Moya, *et al.*, Nature Mater. **13**, 439 (2014).
[2] M. Marathe, *et al.*, Phys. Rev. B **96**, 014102 (2017).
[3] M. Marathe, *et al.*, PSS (b), **1521**, 1700308 (2017).
[4] A. Grünebohm *et al.* Euro. Phys. Lett. **115**, 47002 (2016).

15 min break

KFM 6.4 Mon 16:15 EMH 225

Electronic structure and optical absorption at ferroelectric domain walls in $BiFeO_3$ from first principles — •Sabine Körbel[1,2], Stefano Sanvito[1], and Jirka Hlinka[2] — [1]School of Physics & CRANN, Trinity College, Dublin, Ireland — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic

Recent publications on first principles electronic structure of ferroelectric domain walls (FE DW) in $BiFeO_3$ show some variations concerning existence and magnitude of potential steps and band bending at pristine FE DW. We investigated these properties once more, trying to improve understanding by building on previous works in a systematic way. We also tested the hypothesis that FE DW modify the light absorption properties of $BiFeO_3$.

KFM 6.5 Mon 16:30 EMH 225

Formation of ferroelectric monoclinic domains in $K_{0.7}Na_{0.3}NbO_3$ thin films under different strain conditions — •Leonard von Helden[1], Martin Schmidbauer[1], Michael Hanke[2], and Jutta Schwarzkopf[1] — [1]Leibniz Institute for Crystal Growth (IKZ), Berlin — [2]Paul-Drude-Institute for Solid State Electronics (PDI), Berlin

$K_xNa_{1-x}NbO_3$ is a promising material for lead-free ferro- and piezoelectric applications due to its high piezoelectric and coupling coefficients. Moreover, monoclinic phases - which are favorable as they enable a continuous rotation of the polarization vector - can be induced by incorporating anisotropic epitaxial lattice strain in $K_xNa_{1-x}NbO_3$ thin films. Upon varying the strain conditions the symmetry and orientation of these monoclinic domains can be deliberately tailored as predicted by strain-phase calculations.[1] In order to confirm the theoretical predictions we present a systematic investigation on the ferroelectric domain formation in $K_{0.7}Na_{0.3}NbO_3$ thin films grown by MOCVD. Slightly different strain conditions were realized by the application of various (110) oriented rare earth scandate substrates. The resulting ferroelectric domain structure was investigated upon a combination of piezoresponse force microscopy and X-ray nano-diffraction. Our results reveal monoclinic M_C domains with $(001)_{pc}$ pseudocubic unit cell orientation that differ among the substrates regarding their domain wall inclination. Moreover, the additional occurrence of $(100)_{pc}$ unit cell orientation in films with a thickness above 60 nm will be discussed. [1] J. Schwarzkopf et al., Front. Mater. 4, 26 (2017).

KFM 6.6 Mon 16:45 EMH 225

Phononics at ferroelectric domain walls — •Francesco Foggetti[1,2] and Sergey Artyukhin[1] — [1]Italian Insitute of Technology, Genova, Italy — [2]University of Genova, Italy

Ferroelectric domain walls are emerging as robust 2D systems with promising functionality. Recent scanning tunneling and impedance microscopy studies revealed DC and AC conductivity, 2D electron gas and modified chemistry at ferroelectric domain walls. We study phonons localized at ferroelectric domain walls, and scattering of bulk phonons off ferroelectric domain walls using continuum theory and discrete models.

15 min. break

Invited Talk KFM 6.7 Mon 17:15 EMH 225

Probing STO domain walls with scanning SQUID microscopy — •Beena Kalisky — Department of Physics and Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, Israel

The interface formed by growing LaAlO3 on SrTiO3 (STO), both non magnetic insulators, exhibits conductivity, superconductivity and even magnetism. It is not surprising that the symmetry of the STO substrate is a dominant player in the plethora of physical phenomena found at the interface. We first encountered the interplay between the STO ferroelastic domain walls and the interface while imaging the magnetic flux generated from the interfacial current flow. We found that a big part of the current can be modulated over the STO domain walls and that macroscopic transport measurements are strongly affected. We then investigated the origin of the modulations. We applied local stress to the sample and imaged the change in resistivity. Surprisingly, we found that the resistivity changed mainly along the domain walls which are highly sensitive to pressure. Our study shows that the Scanning SQUID is very useful for the investigation of buried domain walls and their effect on nearby layers.

KFM 6.8 Mon 17:45 EMH 225

LiNbO3 thin-film crystals: A novel class of materials for domain engineering and enhanced domain wall conductivity — •Tillmann Stralka, Alexander Hausmann, Lukas Wehmeier, and Lukas M. Eng — Institute of Applied Physics, Technische Universität Dresden, Germany

In the last years, research on ferroelectric domain wall conductivity (DWC) mostly has focused either on PLD-grown, ultra-thin ferroelectric (FE) films [1] or FE bulk-single crystals [2,3,4]. Here we extend DWC to a novel and extremely prospective class of materials, i.e. freestanding thin-film crystals made up from ultra-thin single-crystalline $LiNbO_3$ (LNO) sheets. We use 5%-Mg-doped LNO polished down to a 22-μm thickness. Beyond high-voltage- [3] and super-bandgap-illumination-induced [4] DW engineering, the sample thinness also allows to write domain patterns by low-voltage AFM lithography, resulting in fully penetrating through domains. Of central interest in these thin-film LNO crystals is the mutual interaction between neighboring DWs, hence providing a novel tool for DW shape engineering on the very local length scale. Investigations are carried out using a combination of AFM techniques (PFM, c-AFM, topography) and Cerenkov Second Harmonic Microscopy [5], as well as by monitoring the electrical transport in DWs along the crystallographic X and Y axes in LNO. [1] J. Seidel et al., Nature Mater. **8** (2009) 229. [2] T. Sluka et al., Nature Comm. **4** (2013) 1808. [3] C. Godau et al., ACS Nano **11** (2017) 4816. [4] M. Schröder et al., Adv. Func. Mater. **22** (2012) 3926. [6] L. Wehmeier et al., Phys. Stat. Solidi **11** (2017) 1700267.

KFM 6.9 Mon 18:00 EMH 225

Correlating domain wall conductivity with geometry: a real-time study via Cerenkov Second Harmonic Generation — •Christian Godau, Lukas Wehmeier, Alexander Haussmann, and Lukas Eng — Institute of Applied Physics, Technische Universität Dresden, D-01062 Dresden, Germany

Ferroelectric domain walls (DWs) have become a central topic of research these days. Especially exploring their electronic properties and domain wall conductivity (DWC) in both thin films [1,2] and single crystals (sc) [3,4,5] has become very attractive. Our recent research on sc-lithium niobate (LNO) has proven an ultra-high DWC [4] and low electronic work function [6] that both provide a solid and promising foundation for prospective electronic device application.

Here, we present a full 3D and time-resolved study by Cerenkov Second Harmonic Generation [7] when investigating the DW dynamics in sc-LNO that are subjected to electric fields. Variations of the field lead to significant changes in geometry and inclination angles of the DW, that is tracked here in real time. These changes in DW-geometry are then correlated to the current measured through the conductive DWs.

[1] J. Seidel et al., Nat. Mater. 8, 229 (2009) [2] S. Cherifi-Hertel et al., Nat. Comm. 8, 15768 (2017) [3] T. Sluka et al., Nat. Comm. 4, 1808 (2013) [4] C. Godau et al., ACS Nano 11, 4816 (2017) [5] M. Schröder et al., Mater. Res. Express 1, 035012 (2014) [6] A.-S. Pawlik et al., Nanoscale 9, 10933 (2017) [7] T. Kämpfe et al., Phys. Rev. B 89, 035314 (2014)

KFM 6.10 Mon 18:15 EMH 225

Domain wall and bulk conductance in $ErMn_{1-x}Ti_xO_3$ — •Theodor Secanell Holstad[1], Donald Malcolm Evans[1], Alexander Ruff[2], Didrik René Småbråten[1], Jakob Schaab[3], Christian Tzschaschel[3], Zewu Yan[4,5], Edith Bourret[5], Sverre Magnus Selbach[1], Stephan Krohns[2], and Dennis Meier[1] — [1]Department of Materials Science and Engineering, NTNU, Norway. — [2]Center for Electronic Correlations and Magnetism, University of Augsburg, Germany. — [3]Department of Materials, ETH, Switzerland. — [4]Department of Physics, ETH, Switzerland. — [5]Materials Sciences Division, UC Berkeley, USA.

Ferroelectric domain walls are attracting broad attention as a novel type of spatially mobile oxide interface that can be written, erased,

and moved on demand. Recently, acceptor and donor doping was adapted to optimize the behavior at ferroelectric domain walls.

In this talk, I will discuss the effect of donor doping on the electronic bulk and domain wall properties in hexagonal $ErMn_{1-x}Ti_xO_3$. Density functional theory calculations show that Ti^{4+} goes to the B-site, replacing Mn^{3+}. Scanning probe microscopy measurements confirm the robustness of the ferroelectric domain template. The electronic transport at both macro- and nanoscopic length scales is characterized. The measurements demonstrate the intrinsic nature of emergent domain wall currents and point towards Poole-Frenkel conductance as the dominant transport mechanism. Aside from the insight into the electronic properties of hexagonal manganites, B-site doping adds an additional degree of freedom for tuning the domain wall functionality.

KFM 7: Microstructure of thin films / TEM-based Nanoanalysis

Time: Monday 15:00–18:20 Location: E 124

KFM 7.1 Mon 15:00 E 124

Scanning Transmission Helium Ion Microscopy on 1nm Thick Carbon Nanomembranes — •Daniel Emmrich[1], Annalena Wolff[2], André Beyer[1], and Armin Gölzhäuser[1] — [1]Bielefeld University, Germany — [2]Queensland University of Technology, Australia

The Helium Ion Microscope (HIM) offers a lateral imaging resolution of 0.3 nm and is known for its excellent sub 10 nm milling capabilities [1]. While imaging with secondary electrons (SE) is well established for this microscope, the ion transmission signal attracts growing attention. Imaging in bright or dark field transmission offers additional information on membranes [2], core shell nanoparticles [3]and can be used for the inspection of milled features, e.g., membrane pores. Monolayer thin membranes have not been studied so far. Here we show a dark field transmission imaging study on 1nm thick Carbon Nanomembrane (CNM) by using a SE conversion plate. CNM are made of self-assembled monolayers that are cross-linked by low energy electrons resulting in a 1 nm thick carbon membrane with tunable conductivity [4]. Imaging the same sample site with different acceptance angles, we are able to compare the measured contrasts with simulated scattering angles from SRIM [5] and discuss the applicability of those simulations on ultimate thin membranes. [1] G. Hlawacek, A. Gölzhäuser (Eds.), Springer Int., Switzerland 2016. [2] A. R. Hall, Microsc Microanal 2013, 19, 740. [3] T. J. Woehl et al., Microsc Anal, 2016, 22, 544. [4] A. Turchanin, A. Gölzhäuser, Adv. Mater 2016, 28, 6075. [5] J. F. Ziegler et al., Nucl. Instr. Meth. Phys. Res. 2010, 268, 1818.

KFM 7.2 Mon 15:20 E 124

Self-assembly of organic semiconducting material at the liquid-liquid interface — •Manuel Johnson, Tim Hawly, and Rainer H. Fink — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058, Erlangen, Germany

Charge transport in organic electronic devices like organic field-effect transistors (OFETs) crucially depends on the structural properties of the active organic layer [1].For their successful preparation homogenous and highly ordered thin films of semiconductor material are required. Since vacuum sublimation induces polycrystalline film growth and therefore limits the performance of thus prepared devices, different solution based techniques have been developed for the fabrication of long-range ordered and single-crystalline organic thin films [2]. We tested a preparation technique where we utilize the self-organization of molecules with sufficiently strong $\pi\pi$-interaction at the liquid-liquid interface and discuss the influence of different preparation parameters. The liquid surrounding offers better chance for molecular diffusion and self-organization and consequently the near-equilibrium growth of crystalline organic films with lateral extensions in the range of several 100um. First microspectroscopic results already confirm the long range order and crystallinity inside the organic thin films.

[1] M. Halik et al, Adv. Mat. 2003, 15
[2] C. Xu, et al., Angewandte Chemie (Intern. Ed.) 55, (2016)

KFM 7.3 Mon 15:40 E 124

Vibrational fingerprints of lithium niobate on insulator and technological aspects for domain inversion in z-cut $LiNbO_3$ thin films — •Peter Mackwitz[1], Michael Rüsing[1], Kai Spychala[1], Minglong Zhai[3], Hui Hu[3,4], 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 — [3]NanoLN, 250101 Jinan, P.R. China — [4]School of Physics, Shandong University, 250100 Jinan, P.R. China

For applications in the field of integrated optics especially lithium niobate on insulator (LNOI) represents a promising layer stack. Here, the outstanding nonlinear optical properties of $LiNbO_3$ and the realizable quasi phase matching via periodic domain inversion can be combined with opportunities from functional layer sequences of thin film lithium niobate and SiO_2. These offer a large built-in vertical refractive index contrast as well as strong confinements. Overall, the LNOI technology offers similar waveguide bending radii and cross-sections as the established silica on insulator technology. Within this work we report on a fundamental characterization of the vibrational properties of lithium niobate on insulator and first steps towards submicron domain inversion in z-cut thin film lithium niobate. In this context a systematic analysis for various annealing conditions interface configurations was performed by confocal Raman-spectroscopy. Furthermore here the successful periodic submicron domain patterning was demonstrated by microscopic and nonlinear imaging.

KFM 7.4 Mon 16:00 E 124

Dopant distribution and octahedral distortions at superconducting complex oxide bilayer interfaces — Y. Eren Suyolcu, Yi Wang, •Wilfried Sigle, Federico Baiutti, Georg Cristiani, Joachim Maier, Gennady Logvenov, and Peter A. van Aken — MPI für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart

We present results of doped lanthanum-cuprate (La2-xMxCuO4 (LMCO), x=0-0.4, M=Ca,Sr,Ba) systems where we systematically varied the dopant ionic radius while the dopant valence state was fixed [1]. Metallic LMCO layers were deposited on LaSrAlO4 followed by a second, insulating La2CuO4 layer, using atomic-layer-by-layer molecular beam epitaxy. Although none of the deposited layers is superconducting individually, the bilayer systems exhibit superconductivity. The critical temperature is found to depend on the dopant species. In order to elucidate possible mechanisms for interfacial superconductivity, the bilayer systems were structurally and chemically characterized in a probe-corrected JEOL JEM-ARM200F microscope. Perfect epitaxial growth is observed and dopants were found to be distributed depending on the dopant size. EELS spectrum imaging shows distinct differences among the three dopant species. Precise measurement of c-lattice parameters shows that the critical temperature is not, as expected, linearly related with the c-lattice parameter, i.e. with the distortion of oxygen octahedral [2]. [1] Y. E. Suyolcu et al., Sci. Rep. 7 (2017) 453. [2] Y. E. Suyolcu et al., Adv. Mater. Interfaces 1700737 (2017).

KFM 7.5 Mon 16:20 E 124

A study on Amorphous Silicon Films using SAXS and SANS to distinguish nano-crystals from voids. — •Eike Gericke[1], Armin Hoell[2], Jimmy Melskens[3], Dragomir Tatchev[4], Uwe Keiderling[2], Robert Wendt[1,2], Simone Raoux[1,2], Klaus Rademann[1], and Klaus Lips[1,5] — [1]Humboldt-Universität Berlin — [2]Helmholtz-Zentrum Berlin — [3]Technische Universiteit Eindhoven — [4]Bulgarian Academy of Sciences — [5]Freie Universität Berlin

Albeit amorphous silicon (a-Si:H) is used since the 70th as thin-film material for opto-electronic applications, its structural properties are still under discussion. a-Si:H contains up to 16 at% of hydrogen in a complex micro- and nano-structured Si-network. Generally, it is described as a continuous random network (CRN), but also models involving nanocrystalls are discussed. TEM hints at nano-voids. It was shown that even reduced-density-functions can be described by a pure CRN but also by a model including nanocrystals. Resolving the complex structure of a-Si:H is essential to correlate light-induced degradation to local inhomogeneities of the material. We revisit the structure of a-Si:H by SAXS and SANS, to distinguish density fluctuations from voids. We have studied differently prepared a-Si:H samples

with morphologies from dense to porous. We will review the structure of a-Si:H and present our results, indicating nano-sized grains with enlarged mass density inside dense- and hydrogen decorated voids inside porous-aSi:H samples. We will present a new model for the a-Si:H structure which correlates the nanostructure with light-induced degradation.

20 min. break

KFM 7.6 Mon 17:00 E 124

New "transrotational" solid state order discovered by TEM in thin films — •Vladimir Kolosov — Ural Federal University, Ekaterinburg, Russia

Exotic thin crystals with unexpected **transrotational** microstructures [1] have been discovered by transmission electron microscopy (TEM) for crystal growth in thin (10-100 nm) amorphous films of different chemical nature (oxides, chalcogenide-based materials, metals and alloys) prepared by various methods. The unusual phenomenon can be observed ***in situ*** in TEM during local e-beam annealing. The dislocation independent regular internal bending of crystal lattice planes in a growing crystal takes place. We call it **transrotation**: unit cell **trans**lation is complicated by small **rotation** realized round an axis lying in the film plane. It can result in strong regular lattice orientation gradients (up to 300 degrees per μm) of different geometries: cylindrical, ellipsoidal, toroidal, saddle, etc. Transrotational microcrystal resembles ideal single crystal enclosed in a curved space. For some geometry types they have bending of atom/lattice planes similar (but much lower) to that of nanotubes and nanonions. Complex skyrmion-like lattice orientation texture is observed in some spherulite crystals. Transrotation is strongly increasing as the film gets thinner. Transrotational micro crystals have been recognized by other authors in some vital thin film materials, i.e. PCMs for memory, silicides, SrTiO3.

[1] V.Yu. Kolosov and A.R.Tholen, Acta Mater., 48 (2000) 1829.

KFM 7.7 Mon 17:20 E 124

Generation of Attosecond Electron Pulse Trains for Ultrafast Transmission Electron Microscopy — •Christopher Rathje[1,3], Katharina E. Priebe[1], Sergey V. Yalunin[1], Armin Feist[1], Thorsten Hohage[2], Sascha Schäfer[1,3], and Claus Ropers[1] — [1]IV. Physical Institute - Solids and Nanostructures, University of Göttingen, Germany — [2]Institute for Numerical and Applied Mathematics, University of Göttingen, Germany — [3]Institute of Physics, University of Oldenburg, Germany

Ultrafast transmission electron microscopy (UTEM) allows for the investigation of dynamics with both nanometer spatial and femtosecond temporal resolution. The highly coherent electron beam of the Göttingen UTEM [1] facilitates detailed studies of inelastic electron-photon scattering [2-4]. Here, we employ intense phase-locked optical fields to coherently control and characterize the longitudinal electron wave function [5]. In particular, we experimentally demonstrate the self-compression of electron pulses due to dispersive pulse propagation into a train of attosecond bursts with peak widths of 655 as [5]. Such pulse trains will enable the study of nanoscale field-driven processes at optical frequencies in UTEM.

[1] Feist et al., Ultramicroscopy 176 (2017) [2] Barwick et al., Nature 462, 902 (2009) [3] Feist et al., Nature 521, 200-203 (2015) [4] Echternkamp et al., Nat. Phys. 12, 1000-1004 (2016) [5] Priebe, Rathje et al., Nat. Photonics 11, 793-797 (2017)

KFM 7.8 Mon 17:40 E 124

Model-based geometry reconstruction of quantum dots from TEM — •Anieza Maltsi[1], Thomas Koprucki[1], Karsten Tabelow[1], and Tore Niermann[2] — [1]Weierstraß-Institut für Angewandte Analysis und Stochastik, Berlin, Germany — [2]Inst. f. Optik und Atomare Physik, TU Berlin, Berlin, Germany

The growth of semiconductor quantum dots (QDs) with desired electronic properties would highly benefit from the assessment of QD geometry, distribution, and strain profile in a feedback loop between growth and analysis of their properties. One approach to assist the optimization of QDs consists in imaging bulk-like samples (thickness 100-300 nm) by transmission electron microscopy (TEM) instead of high resolution (HR) TEM of thin samples (thickness 10 nm). For HRTEM the relaxation of the lamella-like samples may strongly modify the strain field or the preparation may potentially destroy the QDs. However, a direct 3D geometry reconstruction from TEM of bulk-like samples by solving the tomography problem is not feasible due to its limited resolution (0.5-1 nm), the highly nonlinear behavior of the dynamic electron scattering and strong stochastic influences due to uncertainties in the experiment, e.g. excitation conditions. Here, we present a novel concept for 3D model-based geometry reconstruction (MBGR) of QDs from TEM images. The approach includes an appropriate model for the QD configuration in real space, a database of simulated TEM images and a statistical procedure for the estimation of QD properties and classification of QD types based on machine learning techniques.

KFM 7.9 Mon 18:00 E 124

Structural properties of InGaAs Quantum dots investigated by Transmission Electron Microscopy — •Laura Meissner, Tore Niermann, and Michael Lehmann — Technische Universität Berlin, Institut für Optik und Atomare Physik, Straße des 17.Juni 135, Berlin, Deutschland

Optical characteristics of semiconductor quantum dots (QDs) depend closely on their structural properties, like composition, shape, and strain state. By controlling the growth process, these structural properties can be changed and in turn the optical properties are improved. In order to understand the behaviour of the QDs these structural properties have to be monitored.

We report on investigations of composition and strain of InGaAs QDs embedded in GaAs by means of Transmission Electron Microscopy. Microscopic techniques like Geometric Phase Analysis and Dark-field-Electron-Holography are employed to record amplitude and phase of different reflected beams.

In order to avoid relaxation effects and hence observe the strain field of the QDs in a bulk-like state, thick samples (over 100 nm) must be investigated. For these conditions, we discuss the effects of dynamic diffraction on the reflection specific sensitivity to composition and strain.

KFM 8: Multiferroics and magnetoelectrics I (joint session MA/KFM)

Time: Tuesday 9:30–12:15 Location: EB 202

KFM 8.1 Tue 9:30 EB 202

Lu2Fe3O7 a quest for ferroelectricity by charge order — •Sabreen Hammouda and Manuel Angst — Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany.

Rare earth ferrites have attracted a lot of attention as proposed multiferroics. In particular, LuFe2O4 was considered a clear example of ferroelectricity from charge ordering (CO), though recently this was found not to be the case [1]. Structural modification, such as intercalation by LuFeO3, yielding Lu2Fe3O7 might render the bilayers polar. Furthermore, the only believable polarization hysteresis loop in the rare earth ferrite literature [2] was measured on an intercalated compound, slightly Mn-doped Lu2Fe3O7. A critical aspect of investigating these compounds is the oxygen-stoichiometry. We succeeded in growing single crystals of Lu2Fe3O7 using different CO2/CO gas mixtures to fine-tune the oxygen partial pressure. Single crystals examined by x-ray diffraction showed a short range ordering with a zigzagged diffuse scattering along (1/3 1/3 l), with positions similar to the observation by electron diffraction [3]. The diffuse nature indicates that the crystals are not quite stoichiometric enough for long range CO. Powder XRD measurements reveal a peak splitting which is likely due to structural distortion because of CO. Magnetic behavior of these crystals will also be discussed. As an outlook, further optimization is needed to determine the charge and spin structures. [1] de Groot et al., Phys. Rev. Lett. 108, 187601 (2012). [2] Qin et al., Appl. Phys. Lett. 95, 072901 (2009). [3] Yang et al., Phys. Status Solidi B 247, 870 (2010).

KFM 8.2 Tue 9:45 EB 202

Structural and spectroscopic properties of the new mul-

tiferroic Ni_2MnTeO_6 — •Stella Skiadopoulou[1,2], Maria Retuerto[3], Fedir Borodavka[1], Christelle Kadlec[1], Filip Kadlec[1], Zheng Deng[3], Martha Greenblatt[3], Dominik Legut[2], and Stanislav Kamba[1] — [1]Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — [2]VSB Techincal University of Ostrava, Ostrava, Czech Republic — [3]Rutgers, The State University of New Jersey, Piscataway, USA

We present structural, magnetic and spectroscopic studies of a new multiferroic Ni_2MnTeO_6, closely related to the polar antiferromagnet Ni_3TeO_6 known to present a colossal magnetoelectric effect and electromagnons. Single crystals and polycrystalline samples show the same polar structure as Ni_3TeO_6 with the R3 space group down to 4 K. An antiferromagnetic phase transition takes place at approximately T_N=70 K, almost 20 K higher than that of Ni_3TeO_6. This was confirmed by magnetic and dielectric measurements, suggesting the multiferroic character of the compound. Extensive infrared, Raman and THz spectroscopy experiments revealed all phonons predicted by the factor group analysis. THz spectra reveal one new excitation below T_N, which is strongly influenced by external magnetic field, thus assigned to a magnon.

This work was supported by Czech Science Foundation grant No. 17-27790S and Path to Exascale project No. CZ.02.1.01/0.0/0.0/16_013/0001791.

KFM 8.3 Tue 10:00 EB 202

Exotic magnetoelectric excitations of the multiferroic SmFe3(BO3)4 — •Dávid Szaller[1], Artem M. Kuz'menko[2], Alexander A. Mukhin[2], Toomas Rõõm[3], Urmas Nagel[3], Thomas Kain[1], Vlad Dziom[1], Lukas Weymann[1], Alexey Shuvaev[1], Anna Pimenov[1], Vsevolod Yu. Ivanov[2], Irina A. Gudim[4], Leonard N. Bezmaternykh[4], and Andrei Pimenov[1] — [1]Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Prokhorov General Physics Institute, Russian Academy of Sciences, 119991 Moscow, Russia — [3]National Institute of Chemical Physics and Biophysics, Akadeemia tee 23, 12618 Tallinn, Estonia — [4]L. V. Kirensky Institute of Physics Siberian Branch of RAS, 660036 Krasnoyarsk, Russia

Magnetoelectric(ME) multiferroics(MFs), i.e. materials simultaneously hosting ferroelectric and magnetic order, have been attracting enormous interest due to their potential in information-technology applications. Rare-earth ferroborates are a particularly interesting familiy of MF crystals, where the strong spin-orbit interaction at the rare-earth sites results in the coupling of the magnetic and electric degrees of freedom while the ME response is enhanced by the antiferromagnetic ordering of the iron spins. The ME coupling appears in the optical regime as different absorption of counter-propagating light beams, where transparent and dark directions can be swapped by reversing the magnetic field. Furthermore, due to the ME coupling the strength of absorption at spin-wave resonance frequencies can also be tuned by electric field, opening the path for practical applications.

KFM 8.4 Tue 10:15 EB 202

Low energy spin excitations in multiferroic $Mn_2Mo_3O_8$ — •Krisztián Szász[1], Dávid Szaller[2], Sándor Bordács[1], Laur Peedu[3], Johan Viirok[3], Toomas Rõõm[3], Urmas Nagel[3], Vladimir Tsurkan[4], and István Kézsmárki[1,4] — [1]Budapest University of Technology and Economics, Budapest, Hungary — [2]Vienna University of Technology, Vienna, Austria — [3]National Institute of Chemical Physics and Biophysics, Tallinn, Estonia — [4]University of Augsburg, Augsburg, Germany

Recently, it was found that the polar ferrimagnet $Mn_2Mo_3O_8$ shows large diagonal magnetoelectric effect [1]. However, the magnetic structure of this compound is not fully understood. The family of polar ferrimagnets $M_2Mo_3O_8$ with M = Mn, Fe, Co or Ni are excellent materials to investigate the role of different magnetic ions in the microscopic origin of magnetoelectric effect.

In this work magnetization measurements and high magnetic field far infrared spectroscopy are used to unreveal the spin excitations in the low-field ferrimagnetic and in the spin-flop phases. From the magnetic field dependence of the magnon excitation energies we aim to determine the most important exchange and anisotropy parameters. With these parameters it is possible to construct a microscopic spin model of this compound.

[1] T. Kurumaji et al.: PRB 95, 045142 (2017).

KFM 8.5 Tue 10:30 EB 202

Local Magnetic and Electric Interactions in Multiferroic $Ba_2CoGe_2O_7$ and $Sr_2CoSi_2O_7$ — •Martina Schädler[1], Titusz Fehér[2], Norbert Büttgen[1], Vilmos Kocsis[3], Yoshinori Tokura[3], Yasujiro Taguchi[3], and István Kézsmárki[1] — [1]Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany — [2]Department of Physics, Budapest University of Technology and Economics, Hungary — [3]RIKEN Center for Emergent Matter Science, Wako 351-0198, Japan

The multiferroic compound $Ba_2CoGe_2O_7$ has drawn a lot of interest due to its non-centrosymmetric crystal structure, giving rise to peculiar magnetoelectric effects. The spin-dependent hybridization mechanism, that induces the electric polarization, results in a strong coupling of the magnetic moments and the local electric polarization, which allows control of the electric polarization via external magnetic fields. Due to its soft antiferromagnetic structure $Ba_2CoGe_2O_7$ is a promising candidate for tuning the magnetic texture via the application of electric fields. Nuclear Magnetic Resonance (NMR) gives access to the local electric field gradient (EFG) via the nuclear quadrupole moment. We performed ^{59}Co NMR measurements on $Ba_2CoGe_2O_7$ and its sister compound $Sr_2CoSi_2O_7$ in order to determine the local microscopic properties of magnetic spin order and electric polarization at the cobalt site. Through additional application of external electric fields we also investigated the possibility of influencing the local magnetic properties.

15 minutes break

KFM 8.6 Tue 11:00 EB 202

Soft modes in $Ca_3Mn_2O_7$ - Direct observation of the order parameters in a hybrid improper ferroelectric material — •Dirk Wulferding[1,2], Alexander Glamazda[3,1], Peter Lemmens[1,2], Bin Gao[4], Sang-Wook Cheong[4], and Kwang-Yong Choi[5] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]LENA, TU-BS, Braunschweig, Germany — [3]ILTPE, NASU, Kharkov, Ukraine — [4]Rutgers Univ., New Jersey, USA — [5]Chung-Ang Univ., Seoul, Korea

In hybrid improper ferroelectric materials the order parameter is still under debate, but predicted to be a combination of rotation and tilting modes. In the title compound $Ca_3Mn_2O_7$ we observe anomalous softening of rotation and tilting phonons through the transition from the ferroelectric to the paraelectric phase. This clearly underlines their role as order parameters. In addition, a coupling of the soft mode to the magnetic and the electronic subsystems is characterized through an observation of anomalous magnetic and multiphonon Raman scattering. Work supported by the Quantum- and Nanometrology initiative "QUANOMET" within project NL-4, DFG-RTG 1952/1 "NanoMet", Korea NRF Grants (No. 2009-0093817, 2012-046138), and the NSF MRI Grant No. MRI-1532006.

KFM 8.7 Tue 11:15 EB 202

Giant magnetoelectric coupling in the low-dimensional ferrimagnetic iron oxoselenite $Fe_2O(SeO_3)_2$ — •Peter Lemmens[1,2], Vladimir Gnezdilov[3], Dirk Wulferding[1,2], Peter Berdonosov[4], E.S. Kozlyakova[4], E. Kuznetsova[4], Olga Volkova[4], and Alexander Vasiliev[4] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]LENA, TU-BS, Braunschweig, Germany — [3]ILTPE, NASU, Kharkov, Ukraine — [4]MSU, Moscow, Russia

The newly synthesized oxoselenite compound $Fe_2O(SeO_3)_2$ hosts Fe ions in distorted tetrahedral coordination. An anomalous gain in phonon intensity observed within the ferromagnetically ordered phase (T_C = 105 K) hints towards an enhanced electronic polarizability and related giant magnetoelectric coupling. Further anomalous modes of possible magnetic origin are discussed in connection with a strong Dzyaloshinskii-Moriya interaction. Work supported by DFG Project LE967/16-1.

KFM 8.8 Tue 11:30 EB 202

Magnetic and Polar Properties of the Lacunar Spinel $GaMo_4S_8$ — •Korbinian Geirhos[1], Peter Lunkenheimer[1], Hiroyuki Nakamura[2], Yoshikazu Tabata[2], and István Kézsmárki[1] — [1]Experimental Physics V, EKM, University of Augsburg, Germany — [2]Department of Materials Science and Engineering, Kyoto University, Japan

The compound $GaMo_4S_8$ belongs to the family of lacunar spinels AM_4X_8 (A=Ga and Ge; M=V, Mo, Nb, and Ta; X= S and Se). Many of these lacunar spinels exhibit a Jahn-Teller transition associated with ferroorbital ordering. In the so far investigated compounds GaV_4S_8, GaV_4Se_8 and GeV_4S_8, the onset of orbital-order induced

ferroelectricity was found at the Jahn-Teller transition [1,2,3]. Moreover, all of these three materials show strong magnetoelectric coupling with distinct values of the polarization in their magnetically ordered phases, including a skyrmion lattice state, as shown for GaV_4S_8 and GaV_4Se_8 [1, 4]. It was proposed that these skyrmions, which are topologically protected spin textures, carry additional electric polarization [1]. We extend these investigations to another lacunar spinel, $GaMo_4S_8$. The polar properties of this compound were studied by dielectric spectroscopy and pyrocurrent measurements. It shows a Jahn-Teller transition at 47 K, again accompanied by polar ordering. In addition, below 20 K $GaMo_4S_8$ exhibits a complex magnetic phase diagram.

[1] E. Ruff *et al.*, Sci. Adv. **1**, E1500916 (2015). [2] E. Ruff *et al.*, Phys. Rev. B **96**, 165119 (2017). [3] K. Singh *et al.*, Phys. Rev. Lett. **113**, 137602 (2014). [4] Y. Fujima *et al.*, Phys. Rev. B **95**, 180410 (2017)

KFM 8.9 Tue 11:45 EB 202

Ferrimagnetic-type in-gap spin excitations and magnetoelastic coupling in α-$Cu_2V_2O_7$ — •Johannes Werner[1], Liran Wang[1], Alexander Ottmann[1], Robin Weis[1], Mahmoud Abdel-Hafiez[2], Jhuma Sannigrahi[3], Souradip Majumdar[4], Changhyun Koo[1], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg, Germany — [2]Physikalisches Institut, Goethe-Universität, Frankfurt a.M., Germany — [3]ISIS Facility, Rutherford Appleton Laboratory, Didcot, United Kingdom — [4]Department of Solid State Physics, Kolkata, India

Low-energy magnetic excitations and magnetoelastic coupling in multiferroic α-$Cu_2V_2O_7$ have been investigated by high-frequency electron spin resonance (HF-ESR) , thermal expansion, magnetostriction, specific heat and magnetisation studies in magnetic fields up to 15 T. Despite a large antiferromagnetic gap, below 100 GHz we observe low-energy magnetic excitations in the spin ordered phase indicating a ferrimagnetic-type resonance branch associated with the Dzyaloshinsii-Moriya-type canted magnetic moment. The anisotropy parameter $\tilde{D} = 1.3(1)$ meV indicates a sizeable ratio of DM-exchange and magnetic anisotropy. Dilatometry results show negative thermal expansion at $T \leq 200$ K. Pronounced anomalies at $T_N = 35$ K imply coupling to the structure. Failure of Grüneisen scaling confirm that several ordering phenomena are concomitantly driving the multiferroic order. Low-field magnetostriction displays a similar hysteresis loop as the magnetisation which supports the scenario of exchange-striction driven multiferroicity.

KFM 8.10 Tue 12:00 EB 202

Directional dichroism via para-magnetoelectric effect in $Sr_2CoSi_2O_7$ — •Dániel G. Farkas[1], Dávid Szaller[1], Vilmos Kocsis[1,2], Sándor Bordács[1], István Kézsmárki[1], Bence Bernáth[3], Dmytro Kamenskyi[3], Laur Peedu[4], Johan Viirok[4], Toomas Rõõm[4], Urmas Nagel[4], Péter Balla[5], and Karlo Penc[5] — [1]BUTE, Hungary — [2]RIKEN CEMS, Japan — [3]HFML, Netherlands — [4]KBFI, Estonia — [5]WRCP, Hungary

Magnetoelectric multiferroics have been attracting enormous interest due to their potential in information technology applications. An exotic phenomenon, directional dichroism (DD) has been reported for spin excitations in multiferroic melilite single crystals and proposed as a new principle of directional light switches operating in the THz region [1].

Applications of multiferroic compounds seem to be limited to low temperatures where electric and magnetic order coexist. However, recent studies on melilites [2] revealed that an external magnetic field can recover the electric polarization via the para-magnetoelectric effect even above $T_N = 7$ K. Based on these static results we can also expect DD to emerge in the paramagnetic phase of melilites.

Indeed we have found strong DD in the paramagnetic phase of $Sr_2CoSi_2O_7$ in high magnetic field. A simple single-ion model was developed, which described the main features of the high temperature directional dichroism.

[1] I. Kézsmárki, D. Szaller et al. Nat. Commun. 5, 3203 (2013).
[2] M. Akaki et al., Phys. Rev. B 86, 060413(R) (2012).

KFM 9: Skyrmions II (joint session MA/TT/KFM)

Time: Tuesday 9:30–13:15 Location: EB 301

KFM 9.1 Tue 9:30 EB 301

Low temperature magnetic field mapping on Néel-skyrmions in GaV4Se8 — •Franziska Seifert[1], Felix L. Kern[1], István Kézsmárki[2], Daniel Wolf[1], Bernd Büchner[1], and Axel Lubk[1] — [1]Leibniz Institute for Solid State and Materials research Dresden, Germany — [2]University of Augsburg, Germany

Skyrmions are promising candidates for magnetic memory devices, because of their small size, thermal stability and high mobility. Here we report on Skyrmion mapping in GaV4Se8 carried out on our dedicated cryo TEM fitted with a continuous-flow liquid He cryostat, facilitating electron holography and Lorentz TEM down to 7K. Bulk GaV4Se8 is predicted to show Neel type skyrmions below 18K under applied magnetic field between 0.10T and 0.45T mT. Using Lorentz TEM, we characterized the cycloidal and skyrmionic phase of thin GaV4Se8 lamellas in dependence of temperature and applied magnetic field. By mapping the magnetic phase diagram of the thin film we identify magnetic textures that are not considered in the bulk phase diagram. We discuss the origins of these in terms of crystal symmetries and strain prevailing in the thin film slab geometry.

KFM 9.2 Tue 9:45 EB 301

Probing skyrmion lattice phase by NMR in GaV_4S_8 — •Markus Prinz-Zwick, Norbert Büttgen, Vladimir Tsurkan, Martina Schädler, and István Kézsmárki — Center of electronic correlation and magnetism, University of Augsburg

With the discovery of Néel-Type skyrmions forming in a skyrmion lattice (SkL) in the lacunar spinel GaV_4S_8, the characterization and analysis of such polar axially symmetric skyrmion host materials gained general interest. From a microscopic point of view we want to elucidate the local distribution of internal magnetic fields associated with the SkL and probe spin excitations using Nuclear Magnetic Resonance(NMR) spectroscopy. Since the stability of the SkL phase is limited to the sub-Tesla range, this is a highly challenging issue. Here, we report NMR results within the SkL-phase in the lacunar spinel GaV_4S_8, and the first so called zero-field NMR measurements, where the internal field of the V_4 cubanes was exploited to perform ^{51}V measurements for applied magnetic fields $0 < \mu_0 H < 100$ mT.

KFM 9.3 Tue 10:00 EB 301

Optically induced demagnetization and coherent spin excitations in GaV4S8 — •Fumiya Sekiguchi[1], Prashant Padmanabhan[1], Rolf B. Versteeg[1], István Kézsmárki[2], and Paul H. M. van Loosdrecht[1] — [1]Institute of Physics 2, University of Cologne, 50937 Cologne, Germany — [2]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany

Skyrmions are quasiparticle-like topological spin textures stabilized in non-centrosymmetric crystals with Dzyaloshinskii-Moriya interactions. For potential applications and a better understanding of their nature, it is important to understand their creation and annihilation dynamics, as well as their collective excitation spectrum. Here we employ time resolved magneto-optical Kerr experiments to study the magnetization dynamics in the lacunar spinel GaV4S8 which hosts novel cycloid and Néel-type skyrmion magnetic ground states. The experiments show the emergence of a slow demagnetization process in the magnetically ordered states. In addition, we observe coherent collective spin excitations in both the cycloid and skyrmion phases.

KFM 9.4 Tue 10:15 EB 301

Temperature dependence of the cubic anisotropy in the room-temperature skyrmion host $Co_9Zn_9Mn_2$ — •Bertalan György Szigeti[1], Dieter Ehlers[2], Kosuke Karube[3], István Kézsmárki[2], Hans-Albrecht Krug von Nidda[2], Markus Preissinger[2], Vladimir Tsurkan[2], Yusuke Tokunaga[3], Yasujiro Taguchi[3], and Yoshinori Tokura[3] — [1]Department of Physics, Budapest University of Technology and Economics,1111 Budapest, Hungary — [2]Experimental Physik V, EKM, Universität Augsburg, 86135 Augsburg — [3]RIKEN Centre for Emergent Matter Science (CEMS), Wako 351-0198, Japan

The β-Mn-type Co-Zn-Mn alloys are cubic chiral room temperature skyrmion hosts already studied by Lorentz transmission electron microscopy, magnetization and small-angle neutron scattering[1]. Spin wave spectroscopy of the Dzyaloshinskii-Moriya interaction has been measured for $Co_8Zn_8Mn_4$ and $Co_9Zn_9Mn_2$[2]. $Co_9Zn_9Mn_2$ can host metastable skyrmions in zero magnetic field below its $T_C \approx$ 400 K Curie-temperature[3]. In this work we present ESR measurements in the field polarized state of $Co_9Zn_9Mn_2$ to investigate the temperature dependence of the cubic magnetocrystalline anisotropy and its influence on the properties of the meta-stable skyrmion lattice state. We found strong correlation between the change in the anisotropy and the trigonal to square lattice transformation of the skyrmion state.

[1] Tokunaga, Y., et al., Nat. Commun. 6, 7638 (2015), [2] Takagi, R., et al., Phys. Rev. B 95, 220406 (2017), [3] Karube, K., et al., arXiv:1709.08047 (2017).

KFM 9.5 Tue 10:30 EB 301

Effects of Magnetocrystalline Anisotropy on the Triangular to Square Lattice Transformation of Skyrmions — •Markus Preissinger[1], Dieter Ehlers[1], Kosuke Karube[2], István Kézsmárki[1], Hans-Albrecht Krug von Nidda[1], Bertalan Szigeti[3], Yusuke Tokunaga[2], Yasujiro Taguchi[2], Yoshinori Tokura[2], and Vladimier Tsurkan[1] — [1]Experimentalphysik V, EKM, Universität Augsburg, 86135 Augsburg — [2]RIKEN Centre for Emergent Matter Science (CEMS), Wako 351-0198, Japan — [3]Department of Physics, Budapest University of Technology and Economics, 1111 Budapest, Hungary

The β-manganese-type alloy $Co_8Zn_8Mn_4$ exhibits a helical state below the Curie-temperature $T_c \approx 300\,K$ [1]. Below the phase transition, between 300 K and 284 K, an equilibrium skyrmion lattice state occurs in weak magnetic fields in the range of 400 Oe. This state can be quenched down to lower temperatures by rapid field cooling. Below 150 K the metastable triangular skyrmion lattice transforms into a square lattice [2]. The magnetocrystalline anisotropy in the ferromagnetic phase was determined by ferromagnetic resonance measurements. We discuss its impact on the phase transition between the two types of skyrmion lattices. On cooling, the increasing cubic anisotropy constant K_1 seems to drive the phase transition of the skyrmion lattice between 150 K and 40 K. The temperature dependence of the corresponding critical fields turns out to be correlated to the anisotropy constant K_1.

[1] T. Hori et al., J. Magn. Magn. Mater. **310**, 1820–1822 (2007).
[2] K. Karube et al., Nature Materials **15**, 1237–1243 (2016).

KFM 9.6 Tue 10:45 EB 301

Incommensurate magnetic systems studied with the multipurpose three-axis spectrometer (TAS) MIRA at FRM II — •Robert Georgii[1], Tobias Weber[1,2], Georg Brandl[1], and Peter Böni[3] — [1]Maier-Leibnitz Zentrum (MLZ), Garching, Germany — [2]Institut Laue Langevin (ILL), Grenoble, France — [3]Physik Department E21, TU München, Garching, Germany

Incommensurate magnetic structures like Helimagnons and Skyrmions are currently intensively studied. Due to their large size and rigid structure they often show very low-lying excitations, where most of the interesting physics is taking place below some meV. The cold-neutron three-axis spectrometer MIRA is an instrument optimized for such low-energy excitations. Its excellent intrinsic resolution makes it ideal for studying incommensurate magnetic systems. Here we will present several examples for the dynamics of such structures which have been measured with MIRA.

KFM 9.7 Tue 11:00 EB 301

Induction mapping of the 3D Spin Texture of Skyrmions in Thin Helimagnets — •Sebastian Schneider[1,2], Daniel Wolf[1], Matthew J. Stolt[3], Song Jin[3], Darius Pohl[1], Bernd Rellinghaus[1], Marcus Schmidt[4], Bernd Büchner[1], Sebastian T. B. Goennenwein[2], Kornelius Nielsch[1,2], and Axel Lubk[1] — [1]IFW Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]University of Wisconsin-Madison, Madison, USA — [4]MPI CPfS, Dresden, Germany

Envisaged applications of skyrmions in magnetic memory and logic devices crucially depend on the stability and mobility of these topologically non-trivial magnetic textures in thin films. We present for the first time experimental evidence for a characteristic 3D modulation of the skyrmionic spin texture towards the sample surface. Inherent to this structure is the gradual change of the Bloch nature of the skyrmion in the depth of the film to surface chiral twists. By combining focal series inline electron holography (EH), and off-axis EH to quantitatively reconstruct the projected magnetic field pertaining to both the helical and the skyrmion lattice phase in single crystal nanoplates of the isotropic chiral magnet $Fe_{0.95}Co_{0.05}Ge$ nanoplate with electron tomography and magnetostatic simulations of the fields, we extract quantitative information on the 3D spin texture of skyrmions. Our results highlight the relevance of surfaces for the formation of skyrmions in thin film geometries and pave the way towards a surface-induced tailoring of the skyrmion structure.

15 minutes break

Topical Talk KFM 9.8 Tue 11:30 EB 301

Composite topological excitations in ferromagnet-superconductor heterostructures — •Kjetil Hals — Department of Engineering Sciences, University of Agder, 4879 Grimstad, Norway

Heterostructures of conventional superconductors and ferromagnets are currently attracting considerable interest because of their potential use for realizing topological superconductivity. The combination of spin-orbit coupling in the superconductor and the lack of inversion symmetry of these heterostructures leads to a magnetoelectric coupling between the magnetic and superconducting order parameters [1, 2]. In this talk, I demonstrate that the magnetoelectric coupling causes magnetic skyrmions and superconducting vortices to bind, forming skyrmion-vortex pairs (SVPs) which represent topological excitations of the hybrid system [1]. I determine the conditions under which a bound SVP is formed, and characterize the range and depth of the effective binding potential through analytical estimates and numerical simulations. Furthermore, I develop a semiclassical description of the coupled skyrmion-vortex dynamics and discuss how SVPs can be controlled by applied spin currents.

[1] K.M.D. Hals, M. Schecter, M. S. Rudner, Phys. Rev. Lett. 117, 017001 (2016). [2] K. M. D. Hals, Phys. Rev. B 95, 134504 (2017).

KFM 9.9 Tue 12:00 EB 301

Magnetoelectric effect and orbital magnetization in skyrmion crystals: new ways for detection and characterization of skyrmions — •Börge Göbel[1], Alexander Mook[2], Jürgen Henk[2], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle — [2]Institut für Physik, Martin-Luther-Universität, D-06120 Halle

Skyrmions are small magnetic quasiparticles, which are uniquely characterized by their topological charge and their helicity. We present theoretically how both properties can be determined without relying on real-space imaging [1].

The topological Hall effect of electrons allows to distinguish skyrmions from antiskyrmions by sign of the topological Hall conductivity [2,3] and the orbital magnetization [1]. Here, we predict a magnetoelectric effect in skyrmion crystals [1], which is the generation of a magnetization (polarization) by application of an electric (magnetic) field. Its dependence on the skyrmion helicity fits that of the classical toroidal moment of the spin texture and allows to differentiate skyrmion helicities: it is largest for Bloch skyrmions and zero for Néel skyrmions. We predict distinct features in the magnetoelectric polarizability that can be used to detect and characterize skyrmions in experiments.

[1] B. Göbel et al., submitted.
[2] B. Göbel et al., Phys. Rev. B **95**, 094413 (2017).
[3] B. Göbel et al., New J. Phys. **19**, 063042 (2017).

KFM 9.10 Tue 12:15 EB 301

Antiferromagnetic skyrmion crystals: generation and topological spin Hall effect — •Börge Göbel[1], Alexander Mook[2], Jürgen Henk[2], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle — [2]Institut für Physik, Martin-Luther-Universität, D-06120 Halle

Skyrmions are topologically nontrivial, magnetic quasi-particles, that are characterized by a topological charge. A regular array of skyrmions—a skyrmion crystal (SkX)—features the topological Hall effect (THE) of electrons [1,2], that, in turn, gives rise to the Hall effect of the skyrmions themselves.

We present a generally applicable method to create stable antiferromagnetic skyrmion crystals (AFM-SkXs) by growing a two-sublattice SkX onto a collinear antiferromagnet. As an example we show that both types of skyrmion crystals—conventional and antiferromagnetic—exist in honeycomb lattices. While AFM-SkXs do

not show a THE, they exhibit a topological spin Hall effect [3]. The zero skyrmion Hall effect carries over to isolated AFM skyrmions as well. They can move in straight lines, at higher velocities and need lower driving currents compared to conventional skyrmions [4,5].

[1] B. Göbel et al., Phys. Rev. B **95**, 094413 (2017).
[2] B. Göbel et al., New J. Phys. **19**, 063042 (2017).
[3] B. Göbel et al., Phys. Rev. B **96**, 060406(R) (2017).
[4] J. Barker et al., Phys. Rev. Lett. **116**, 147203 (2016).
[5] X. Zhang et al., Sci. Rep. **6**, 24795 (2016).

KFM 9.11 Tue 12:30 EB 301

Topological Hall effect in Heusler compound $Mn_{1.4}PtSn$ — •Praveen Vir, Nitesh Kumar, Chandra Shekhar, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Skyrmions are topologically stable vortex-like spin structure which are considered as potential candidate for future high density memory devices. They have been detected in many chiral and polar compounds such as MnSi, FeGe, Co-Mn-Zn, GaV_4S_8 etc. Recently, with the help of Lorentz transmission electron microscopy, one new vortex like spin structure, so called antiskyrmions have been discovered in Mn-based tetragonal Heusler compound $Mn_{1.4}PtSn$ and $Mn_{1.4}Pt_{0.9}Pd_{0.1}Sn$ [1]. Antiskyrmion has been predicted to be anti-particle of Néel or Bloch type skyrmions becuase they annihilate with conventional skyrmions [2]. They are also topologically stable and consist of topological winding number or skyrmion number +1 [3]. Due to this topologically stable spin nature, it can give rise to non-vanishing Berry phase in real space. In other words, there could be nonzero topological Hall effect. Here, we report large topological Hall effect in single crystal of antiskyrmion hosting compounds $Mn_{1.4}PtSn$.

KFM 9.12 Tue 12:45 EB 301

Prospecting anti-skyrmions in ultra-thin Co films deposited on W(110) — •Flaviano José dos Santos, Bernd Zimmermann, Stefan Blügel, Manuel dos Santos Dias, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

Recently, the possibility of anti-skyrmion formation in magnetic films on substrates with low symmetry due to anisotropic Dzyaloshinskii-Moriya interactions (DMI) has been demonstated [1]. Experimentally, such anisotropic DMI has been found for Co-films on W(110) [2]. Motivated by these findings, we investigated from first-principles the tensor of magnetic interactions of films containing up to three layers of Co reconstructed on W(110) surface as a continuation of our previous study [3]. We use the full-potential relativistic Korringa-Kohn-Rostoker Green function method combined with a technique employing infinitesimal rotations to access the different components of the tensor. The anisotropy, magnitude and sign of the interactions are analysed in detail with a focus on the DMI. Using atomistic spin dynamics simulations, we prospect and demonstrate the existence of skyrmions and anti-skyrmions, which depend strongly on the thickness of Co films. Finally, we unveil the spin-wave excitations characterising the topologically distinct skyrmionic objects.

Work supported by the Brazilian agency CAPES (Project No. 13703/13-7) and the European Research Council (ERC-consolidator Grant No. 681405-DYNASORE). [1] Nat. Commun. 8, 308 (2017); [2] Phys. Rev. B 95, 214422 (2017); [3] Phys. Rev. B 95, 134408 (2017).

KFM 9.13 Tue 13:00 EB 301

Material systems for skyrmions in Co-based ferro-/antiferromagnetically (FM/AFM) coupled multilayers — •Hongying Jia, Bernd Zimmermann, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Magnetic skyrmions, in particular AFM skyrmions, are considered as ideal candidates for high storage density information carriers due to the suppressed skyrmion Hall effect and a smaller size by canceling the dipolar fields. So far searching for materials that can host AFM skyrmions is still a challenging task. Magnetic multilayers (MMLs) with composite structures provide a great opportunity to design materials that can host spin-spirals, skyrmions or magnetic domains with optimal properties. Here we will present the qualitative trends of magnetic exchange interactions throughout a wide range of $\{Z|\mathrm{Co}|\mathrm{Pt}\}$ MMLs (Z=3d: Cu, Zn; 4d: Tc∼Cd; 5d: Au). The AFM coupling in between the Co layers was observed in $\{Z|\mathrm{Co}|\mathrm{Pt}\}$ MMLs (Z=Zn, Ru, Rh, Cd). The effects of 3d-4d-5d hybridization between Co and the nonmagnetic metals, in particular the effects around the Fermi level, on the magnetic interactions will be discussed. The correlation between the electric interface dipole moments and the sign and magnitude of the Dzyaloshinskii-Moriya interaction will be also discussed.

We acknowledge financial support from the MAGicSky Horizon 2020 European Research FET Open project (#665095) and computing time at JURECA from Jülich Supercomputing Center and JARA-HPC.

KFM 10: Spectroscopy and Microscopy I with X-rays and Ions

Chair: Burkhard Beckhoff - Physikalisch-Technische Bundesanstalt, Berlin, Germany

Time: Tuesday 9:30–13:40 Location: EMH 225

Invited Talk KFM 10.1 Tue 9:30 EMH 225

Insights into the Inside provided by Coherent X-ray Imaging — •Tim Salditt — Georg-August-Universität Göttingen, Institut für Röntgenphysik, Friedrich-Hund-Platz 1, 37077 Göttingen

X-rays can provide information about the functional architecture of materials, including soft and biological matter [1 ,2], also in a heterogeneous state and in operando [3]. However, the specific advantages of hard x-rays in view of penetration power, high spatial resolution, quantitative contrast, and compatibility with environmental conditions is to date not fully exploited, mainly due to shortcomings in x-ray optics. With the advent of highly brilliant radiation, coherent focusing, and lens-less diffractive imaging this situation has begun to change. Nanofocused coherent x-ray synchrotron beams are now routinely used for scanning as well as for full field holographic x-ray imaging, in 2d and 3d. Even 4d movies of materials [4] are enabled by time-resolved tomography, providing new insights into the inside of materials as well as functional processes. In this talk I present the optical concepts and challenges, including phase retrieval and image reconstruction, and explain all the buss about holography, ptychography and tomography.

[1] M. Bartels, M. Krenkel, J. Haber, R. N. Wilke, and T. Salditt, Phys. Rev. Lett. (2015), 114, 048103. [2] M. Töpperwien, M. Krenkel, D. Vincenz , F. Stöber, A. M. Oelschlegel, J. Goldschmidt and T. Salditt, Scientific Reports (2017), 7, 42847. [3] J. Wallentin, M. Osterhoff and T. Salditt, Adv. Mater. (2016), 28, 1788. [4] A. Ruhlandt, M. Töpperwien, M. Krenkel, R. Mokso, and T. Salditt, Scientific Reports (2017), 7, p. 6487.

KFM 10.2 Tue 10:00 EMH 225

Laboratory soft X-ray Tomography — •Aurélie Dehlinger[1,2], Julia Bränzel[1,3], Daniel Grötzsch[1,2], Robert Jung[3], Birgit Kanngiesser[1,2], Stefan Rehbein[4], Christian Seim[5], and Holger Stiel[1,3] — [1]Berlin Laboratory for innovative X-ray technologies (BLiX) — [2]Technische Universität Berlin, Institut für Optik und Atomare Physik, Hardenbergstr. 36, 10623 Berlin, Germany — [3]Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin, Germany — [4]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Straße 15, 12489 Berlin, Germany — [5]Physikalisch-Technische Bundesanstalt, Abbestr 2-12, 10587 Berlin, Germany

In microscopy, where the resolution depends on the wavelength of the probing light, soft X-rays can be used to analyze samples that cannot be resolved with visible light microscopes. X-ray microscopy in the water window allows imaging with resolutions in the nanometer regime as well as a high contrast between carbon and oxygen, which is an ideal condition for the tomographic investigation of biological samples in their natural state. We present a Full-Field Laboratory Transmission X-ray Microscope (LTXM) at the Berlin Laboratory for innovative X-ray technologies (BLiX) with a probing radiation energy of 500 eV, provided by a laser-based nitrogen plasma source. The development of laboratory X-ray sources aims to increase the availability of X-ray microscopy to a broader scientific community. We will present the latest

measurements carried out on biological samples and the corresponding reconstructed tomograms, which are the key to a more precise and global analysis in various fields of life science.

KFM 10.3 Tue 10:20 EMH 225

Tomography with extended sources — •Leon Merten Lohse, Malte Vassholz, and Tim Salditt — Institut für Röntgenphysik, Friedrich-Hund-Platz 1, 37077 Göttingen, Deutschland

X-ray computed tomography (CT) is widely used today for nondestructive 3D imaging. In practice, the achievable resolution for analytical CT in the laboratory is still limited by the low brilliance of table top sources. One way to overcome this limitation is the use of a line source, as has been demonstrated recently [2]. The larger x-ray source spot allows more photons to contribute to image formation. It has been shown that a reconstruction scheme based on the 3D Radon transform is in fact compatible with a line source and the impact on the resolution can be controlled to be minor [1]. As the method allows to increase the flux at constant resolution, it promises to overcome the trade-off between acquisition time and resolution, and ultimately to allow higher resolutions in laboratory-based analytical CT.

[1] L. M. Lohse et al. "Tomography with extended sources: ...", Phys. Rev. A (accepted 11/2017) [2] M. Vassholz et al. "New X-Ray Tomography Method ... ", Phys. Rev. Lett. (2016)

KFM 10.4 Tue 10:40 EMH 225

Imaging with Nanometer Resolution from 8 to 100 keV using Multilayer Zone Plates (MZP) — •Jakob Soltau, Tim Salditt, and Markus Osterhoff — Institut für Röntgenphysik, Georg-August-Universität Göttingen, Göttingen, Germany

The brilliance of modern synchrotrons cleared the path towards generating highly focussed x-ray beams. Latest developments in the fabrication of multilayer zone plates (MZP) using the pulsed laser deposition process have enabled to decrease the resolution defining smallest zone widths down to 5 nm [1]. At the same time the optical thickness, important for efficiency, was enlarged up to 30 μm. In recent experiments at Petra III endstation P10, the MZPs were used in a scanning microscopy setup at 13.8 keV. It was possible to resolve a Siemens star test pattern with smallest feature sizes of 50 nm. A first proof-of-concept experiment at the ESRF endstation ID31, extended the limit of imaging with MZPs to photon energies of 100 keV [2].

[1] C. Eberl et al. Fabrication of laser deposited high... In: Applied surface science 307 (2014)

[2] M. Osterhoff, et al. , Ultra-high-aspect multilayer zone plates for even higher x-ray energies, Proc. SPIE (2017)

KFM 10.5 Tue 11:00 EMH 225

Divide and Update: Towards Single-Shot Object and Probe Retrieval for Near-Field Holography — •Johannes Hagemann[1,2] and Tim Salditt[1] — [1]Institut für Röntgenphysik, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]current address: DESY, X-Ray Nanoscience and X-Ray, Optics, Notkestraße 85, 22607 Hamburg

We present a phase reconstruction scheme for X-ray near-field holographic imaging based on a separability constraint for probe and object. In order to achieve this, we have devised an algorithm which requires only two measurements – with and without an object in the beam. This scheme is advantageous if the standard flat-field correction fails and a full ptychographic dataset can not be acquired, since either object or probe are dynamic. The scheme is validated by numerical simulations and by a proof-of-concept experiment using highly focused undulator radiation of the beamline ID16a of the European Synchrotron Radiation Facility (ESRF).

KFM 10.6 Tue 11:20 EMH 225

Multiskalige Analyse von Energiematerialien mittels Synchrotron und Focused Ion Beam — •Markus Osenberg[1], André Hilger[2], Henning Markötter[2], Tobias Arlt[1], Thomas Turek[3], Volker Schmidt[4], Joachim Binder[5], Ingo Manke[2] und John Banhart[1,2] — [1]Technische Universität Berlin — [2]Helmholtz-Zentrum Berlin — [3]Technische Universität Clausthal — [4]Universität Ulm — [5]Karlsruhe Institute of Technology

Forschung an Energiematerialien rückt immer mehr in den Fokus und gerade das Wissen über die zu Grunde liegenden, inneren Strukturen dieser Materialien, ist von entscheidender Bedeutung für die Weiterentwicklung. Energiematerialien wie zum Beispiel Batterie-, Elektrolyseelektroden oder mikroporöse Diffusionslagen aus der Brennstoffzellenindustrie wurden sowohl auf der Mikrometer als auch auf der Nanometerskala tomografiert und analysiert. Dazu wurden zum einen, hochauflösende Synchrotronmessungen am BESSY II und Focused Ion Beam (FIB) Messungen am Helmholtz-Zentrum Berlin durchgeführt. Außerdem wurden auf der Nanometerskala 2D Untersuchungen gemacht, um die Messmethoden besser miteinander verknüpfen zu können. Besonders die FIB-Messungen standen hier im Fokus bezüglich der Probenpräparation und der artefaktfreien Rekonstruktion. Auf Grundlager dieser multiskaligen Messungen konnten Zusammenhänge zwischen Herstellungsparametern und Morphologie der Materialien gezeigt werden. Darüber hinaus führten die Analysen dieser Messungen zu einem tieferen Verständnis des Rekonstruktionsprozesses von FIB-Daten und somit zu präziseren Repräsentationen der vermessenen Proben.

20 min. break

KFM 10.7 Tue 12:00 EMH 225

Simulation of Large Solid Angle Effects for XRF Quantification - First Results — •Hanna Dierks[1], Lars Lühl[1], Konstantin Andrianov[2], Thomas Wilhein[2], and Birgit Kanngiesser[1] — [1]AG Kanngießer, IOAP/TU Berlin — [2]Institute for x-optics, Hochschule Koblenz

Soft and tender X-ray microscopy (XRM) at cellular level is used worldwide to investigate biomedicine samples. Scanning transmission X-ray microscopy (STXM) in combination with fluorescence detection is able to map elements from C to Mo with a lateral resolution below 100 nm. Since biological samples generally emit rather weak fluorescence signals, a high detector efficiency (e.g large solid angle) is necessary to avoid long measurement times. The AnImaX endstation is equipped with a new annular QUAD detector which yields a very large solid angle of detection (up to 1.2 sr). Established quantification approaches normally assume a small detector area with respect to the distance sample to detector, limiting the solid angle. For large solid angles, new effects occur, since the detected radiation passes a wide angular range on its way out of the sample. This results in geometrically different exit path lengths and, for inhomogeneous samples, even different sample composition (resp. absorption coefficients). In the following, these effects are simulated based on the Sherman equation combined with an additional virtual decomposition of the sample and detector. These forward calculations aim as a first step towards the development of new quantification concepts for annular detectors with a large solid angle.

KFM 10.8 Tue 12:20 EMH 225

Scanning Transmission X-ray Microscopy with Fluorescence Detection — •Andreas Haidl[1], Konstantin Andrianov[1], Thomas Nisius[1], Lars Lühl[2], Aurelie Dehlinger[2], Hanna Dierks[2], Birgit Kanngiesser[2], and Thomas Wilhein[1] — [1]Institute for X-Optics, University of Applied Sciences Koblenz, RheinAhrCampus Remagen, Germany — [2]Institute for Optics and Atomic Physics, Technical University Berlin, Germany

X-ray microscopy can be used in many research fields for imaging applications with resolutions notable below 100nm, continuously pushing the limits to near diffraction limited resolutions.

AnImaX (Analytical Imaging with X-rays) is a flexible endstation for combining scanning and full field microscopy using synchrotron radiation in the soft X-ray spectral range. The AnImaX platform consists out of up to three separate vacuum chambers and custom designed high resolution piezo driven stages. The AnImaX endstation has been successfully put to work at the beamline P04 at PETRA III.

The use of a spatial resolved detector in scanning mode allows the simultaneous acquisition of different imaging modes by adjusting the detector response function. The CCD based multimodal detector system allows beside absorption contrast the acquisition of phase contrast and dark field images. The obtained diffraction patterns can also be used for ptychography. In the scanning mode the SDD detector with its outstanding solid angle of detection also gathers a fluorescence spectrum for each pixel. Thereby a detailed spatial elemental and chemical analysis of the specimen is performed.

KFM 10.9 Tue 12:40 EMH 225

LABORATORY(CONFOCAL) MICRO-XRF ON CRYO-FIXATED BIOLOGICAL SPECIMEN — •Frank Förste, Tobias Drechsel, Ioanna Mantouvalou, and Birgit Kanngiesser — IOAP TU Berlin, Hardenbergstraße 36, 10623 Berlin

The non-destructive imaging of elemental distributions in specimen is

of high interest in many fields of research as for example in biology, geology or archaeometry, when sectioning or sampling is undesirable. In biology, specimen have a high content of water, which leads to the challenge, that specimen must be fixated to stop a change in elemental distributions due to drying or shrinking during measurements. Most commonly specimens are either freeze-dried or cryo-fixated, the latter being the method of choice regarding the maximal sample integrity. X-ray fluorescence (XRF) techniques like micro-XRF (up to 2D) or confocal micro-XRF (up to 3D) can easily be combined with a cryogenic sample environment, thus, fulfilling the above-mentioned requirements for elemental imaging of biological specimen. In this work, a modified commercial micro-XRF spectrometer (M4 Tornado, Bruker Nano GmbH) is used [1]. The instrument enables micro-XRF as well as confocal micro-XRF with high speed acquisition and lateral resolutions of 30 *m at Cu Kα. We present the addition of a liquid nitrogen Cryo-Jet (Oxford Instruments) which cools the specimen to 120 K rendering longtime measurements of biological specimen feasible. Characterization and stability measurements show the feasibility for cryomeasurements in the laboratory. As a first application, sunflower roots which show different uptake of heavy metals are investigated.

KFM 10.10 Tue 13:00 EMH 225

micro-XRF analysis of color brilliance and dyeing techniques in ancient wool carpet fibers — •Andreas Späth[1], Markus Meyer[1], Thomas Huthwelker[2], Camelia N. Borca[2], Karl Messlinger[3], Manfred Bieber[4], and Rainer H. Fink[1] — [1]1FAU Erlangen-Nuremberg, Physical Chemistry II, Erlangen, Germany — [2]Paul Scherrer Institute, Swiss Light Source, Villigen, Switzerland — [3]FAU Erlangen-Nürnberg, Physiology and Pathophysiology, Erlangen, Germany — [4]Ex Oriente, Waldbrunn, Germany

The vivid and persisting colors of ancient oriental carpets are remarkably stable against any typical form of bleaching. Anthropologists have revived traditional procedures based on fermentation of the wool with G. candidum yeast prior to dyeing. This method results in a higher permeability of the fiber cuticle, but in ancient wool specimens the cuticles are often lost by abrasion and cannot be analyzed anymore. However, the common natural dyes (e.g., alizarin) require the use of a mordant (KAl(SO4)2 or FeSO4) to form a stable mordant-dye-coordination-complex within the keratin fiber. micro-XRF is an excellent tool to detect the distribution of the respective mordant-dye-complexes within the wool [1]. We found that fermentation results in an enhanced concentration of mordant in the inner cortex. Within our recent studies we employ micro-XRF to confirm the fermentation process in specimens from various centuries and cultures - including the oldest knotted carpet known (5th century B.C.) - and gain more insight into the historical spreading of this technique.

[1] M. Meyer et al., Scanning, 2017, 2017, 6346212.

KFM 10.11 Tue 13:20 EMH 225

Applicability of a Laboratory Scan-Free GEXRF Setup for the Investigation of Nano-Layered Samples — •Veronika Szwedowski, Jonas Baumann, Steffen Staeck, Gesa Goetzke, Ioanna Mantouvalou, Daniel Groetzsch, Wolfgang Malzer, and Birgit Kanngiesser — Institut für Optik und Atomare Physik, BLiX, Technische Universität Berlin, Deutschland

Grazing Emission X-Ray Fluorescence (GEXRF) is an analytical method enabling access to information about elemental depth gradients, diffusion or doping profiles of nanoscale samples. A novel scan-free approach significantly simplifies GEXRF setups by using a position and energy dispersive detector, avoiding movable parts in the spectrometer.

The first demonstrations of the technique were shown using synchrotron radiation or laser-produced plasma sources in combination with high-prized detectors enabling fast and stable angle dependent XRF measurements.

In this work a Scan-Free GEXRF (SF-GEXRF) setup with a microfocus rhodium X-Ray tube and a conventional CCD is introduced which will help to widen the applicability of the technique due to its simplicity and low-cost, while maintaining high efficiency. We show the investigation of two classes of multilayer samples with layer thicknesses in the low-nanometer to sub-nanometer range.

KFM 11: Dielectric, Elastic and Electromechanical Properties

Time: Tuesday 10:00–11:40 Location: EMH 025

KFM 11.1 Tue 10:00 EMH 025

Optical properties of titanium-doped lithium niobate from time-dependent density-functional theory — •Michael Friedrich[1], W. G. Schmidt[1], Arno Schindlmayr[1], and Simone Sanna[2] — [1]Department Physik, Universität Paderborn, 33095 Paderborn, Germany — [2]Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen

Lithium niobate ($LiNbO_3$) is a dielectric crystal with outstanding electro-optical properties that is widely used for optical waveguides and other commercial applications. The usage in waveguides is made possible by titanium indiffusion. Although this technique has been used for decades, the underlying microscopic processes during indiffusion and the definite lattice sites that are occupied by titanium are insufficiently known to this day.

We model the properties of pristine and titanium-doped $LiNbO_3$ from first principles. The dielectric functions are calculated within time-dependent density-functional theory, and a model long-range contribution is employed for the exchange-correlation kernel in order to account for the electron-hole binding. Our study focuses mainly on the influence of substitutional titanium atoms on lithium sites. We show that an increasing titanium concentration enhances the values of the refractive indices and the reflectivity [1]. This effect cannot be observed by titanium atoms occupying niobium sites.

[1] M. Friedrich *et al.*, Phys. Rev. Materials **1**, 034401 (2017).

KFM 11.2 Tue 10:20 EMH 025

Characterization of extremely small nonlinearities of dielectric response in glasses and glass ceramics — •Florian Bergmann[1,2], Martin Letz[1,2], Gerhard Jakob[2], and Holger Maune[3] — [1]Schott AG, Mainz, Germany — [2]Johannes Gutenberg Universität, Mainz, Germany — [3]Technische Universität, Darmstadt, Germany

Recent mobile network solutions require better microwave circuit performances than ever before. Material solutions need to tackle the challenge of intermodulation between high power signals, e.g. the sending channels of a microwave base station. Intermodulated signals can interfere with the receiving channel with orders of magnitude lower intensity. Therefore, also these very weak passive intermodulation (PIM) levels need to be controlled. One source of intermodulation is the nonlinear response of dielectrics to the electric field. However, there exists only few experimental data on the characterization of nonlinear dielectrics in the GHz frequency range with a sensitivity necessary for mobile communication solutions. Following a resonator method (1) exciting eigenresonances of three coupled cylindrical dielectric resonators enables to measure nonlinear behavior at high field strengths and allow isolating the resonators' material nonlinearities from other intermodulation sources. We report on the latest progress on determining the nonlinear response of glass and glass-ceramics.

(1) T. Nishikawa et al. 'Third harmonic distortion of dielectric resonator material' Jpn. J. Appl. Phys. 28, 2528-31, (1989).

KFM 11.3 Tue 10:40 EMH 025

Sequential polarization switching in ferroelectrics* — •Ruben Khachaturyan — Technische Universität Darmstadt, Darmstadt, Germany

The classical Kolmogorov-Avrami-Ishibashi (KAI) statistical theory of polarization reversal in a uniform ferroelectric medium proved to be a widely used tool in polarization kinetics description. However, based on independent nucleation mechanism the model is not able to describe subsequent events such as 90°-switchings which follow each other. Such 90°-switchings were established experimentally by in situ x-ray diffraction measurements and ultrasonic investigations.

In this work, we expand the KAI model to describe also sequential 90°-switchings. The model explains well recent experimental results of simultaneous time-resolved macroscopic measurements of polarization and strain, performed on a tetragonal Pb(Zr,Ti)O3 ceramic.

Results of simulation allow us to distinguish between 90°- and 180°

switchings, estimate their shares as well as to determine characteristic switching times of these processes, and their activation fields.

KFM 11.4 Tue 11:00 EMH 025

Dielectric Response - Answer to Many Questions in the Methylammonium Lead Halide Solar Cell Absorbers — •Doru C. Lupascu[1], Irina Anusca[1], Šarunas Svirskas[2], Pascale Gemeiner[3], Mehmet Sanlialp[1], Gerhard Lackner[1], Christian Fettkenhauer[1], Jaroslavas Belovickis[2], Vytautas Samulionis[2], Maksim Ivanov[2], Brahim Dkhil[3], Juras Banys[2], and Vladimir V. Shvartsman[1] — [1]Universität Duisburg-Essen, Essen, Deutschland — [2]Vilnius University, Vilnius, Lithuania — [3]Centralesupelec, Gif-sur-Yvette, France

Hybrid organic-inorganic perovskites CH3NH3PbX3 (X = I, Br, Cl) can potentially revolutionize the world of solar cells. The origin of the exceptionally large diffusion length of their photogenerated charge carriers, that is, their low recombination rate, remains elusive. We show that the dielectric constant conserves very high values (>27) for frequencies below 1 THz in all three halides. This efficiently prevents photocarrier trapping and their recombination owing to the strong screening. Similarly large contributions to the dielectric constant are attributed to the dipolar disorder of the CH3NH3+ cations as well as lattice dynamics in the Gigahertz range yielding dielectric constants of $\epsilon = 62$ for the iodide, 58 for the bromide, and about 45 for the chloride below 1 GHz at room temperature. Disorder continuously reduces for decreasing temperature. Dipole dynamics prevail in the intermediate tetragonal phase. The low-temperature orthorhombic state is antipolar. No indications of ferroelectricity are found.

KFM 11.5 Tue 11:20 EMH 025

On the Theory of Magneto-Optical Effects in Crystalline Dielectrics — •Nadine Suzan Cetin, Marius Dommermuth, and Nils Schopohl — Institut für Theoretische Physik and CQ Center for Collective Quantum Phenomena and their Applications in LISA$^+$, Eberhard-Karls-Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen, Germany

A recent theory of the propagation of light in crystalline dielectrics, based on an exact solution of the fundamental field integral equations determining the microscopic local electric field, solely with the individual microscopic polarizabilities $\alpha(\mathbf{R},\omega)$ of atoms (molecules, ions) at a site $\mathbf{R}$ and the crystalline symmetry as input into the theory[1], is extended to take into account the effects of a static external magnetic induction field $\mathbf{B}^{(0)}$ within a Lorentz oscillator model. Decomposing the microscopic local electric field into longitudinal and transversal parts, an effective wave equation determining the radiative part of the macroscopic field in terms of the transverse dielectric tensor $\varepsilon_{ab}^{(T)}\left(\mathbf{q},\omega;\mathbf{B}^{(0)}\right)$ is deduced from the exact solution to the field-integral equations. The Taylor expansion $\varepsilon_{ab}^{(T)}\left(\mathbf{q},\omega;\mathbf{B}^{(0)}\right) = \varepsilon_{ab}^{(T)}(\omega) + i\gamma_{abc}(\omega)\,q_c + \alpha_{abcd}(\omega)\,q_c q_d + A_{abc}^{(1)}(\omega)\,B_c^{()} + A_{abcd}^{(1)}(\omega)\,B_c^{(0)} q_d + \ldots$ around $\mathbf{q} = \mathbf{0}$ and around $\mathbf{B}^{(0)} = \mathbf{0}$ provides then insight into various optical and magneto-optical phenomena, in full agreement with the phenomenological reasoning of Agranovich and Ginzburg. We present calculations of the Faraday effect for quartz, CaF_2 and BaF_2 and compare with experimental data.

[1] Marius Dommermuth and Nils Schopohl, arXiv:1709.07277

KFM 12: Multiferroics and magnetoelectrics II (joint session MA/KFM)

Time: Wednesday 9:30–12:00 Location: EB 202

KFM 12.1 Wed 9:30 EB 202

Magneto-ionic ON/OFF switching of magnetization in FeOx/Fe nanostructures — •Jonas Zehner, Kenny Duschek, Nicolas Peréz, Andreas Petr, Rudolph Schäfer, Kornelius Nielsch, and Karin Leistner — IFW Dresden

A novel route towards low-power voltage-control of magnetism was recently discovered by utilizing voltage-induced ion migration and electrochemical oxidation/reduction in oxide/metal films and denominated magneto-ionic effect [1,2,3]. In all-solid architecture, significant magneto-ionic effects are achieved at elevated temperatures when ion migration is thermally activated. Instead, we present large voltage-induced magnetic changes within several nanometers of FeOx/Fe films at room temperature. The voltage is applied via a liquid alkaline electrolyte [4] (KOH or LiOH solution), which, in comparison to solid oxide gate barrier layers, yields an enhanced electric field and a higher ion mobility at the electrode surface. Nearly complete and reversible voltage-induced ON/OFF switching of magnetization (up to 90 %) is observed in granular FeOx/Fe thin films for a voltage change of 1 V, proven by in situ AHE and in situ FMR. An in situ Kerr microscope set-up has been developed that resolves magnetic domains through a liquid alkaline electrolyte. Thereby, for the first time, the study of the local impact of electrochemical reactions on the magnetic domain characteristics becomes possible for solid/liquid magneto-ionic systems. [1] Song et al., Prog. Mater Sci. 87, 33, 2017, [2] Leistner et al., Phys.Rev. B 87, 224411, 2013, [3] Bauer et al., Nat. Mater. 14, 174, 2015, [4] Duschek et al., APL Mater. 4, 032301, 2016

KFM 12.2 Wed 9:45 EB 202

Magnetoelectric memory function with optical readout — Vilmos Kocsis[1,2], Karlo Penc[2,3], Toomas Rõõm[4], Urmas Nagel[4], •Jakub Vít[2,5], Judit Romhányi[6], Yusuke Tokunaga[1], Yasujiro Taguchi[1], Yoshinori Tokura[1], István Kézsmárki[2,7], and Sándor Bordács[2] — [1]RIKEN CEMS, Japan — [2]Budapest University of Technology and Economics, Hungary — [3]HAS, Hungary — [4]NICPB, Estonia — [5]Institute of Physics ASCR, Czech Republic — [6]OISTGU, Japan — [7]EP5, University of Augsburg, Germany

The ultimate goal of multiferroic research is the development of new generation non-volatile memory devices, the so-called magnetoelectric (ME) memories, where magnetic bits are controlled via electric fields without the application of electrical currents, being subject to dissipation. This low-power operation exploits the entanglement of the magnetization and the electric polarization coexisting in multiferroic materials. Here I will demonstrate the optical readout of ME memory states in the antiferromagnetic (AFM) and antiferroelectric (AFE) $LiCoPO_4$, based on the strong absorption difference of THz radiation between its two types of ME domains. [1] This unusual contrast is attributed to the dynamic ME effect of the spin-wave excitations, as confirmed by our microscopic model, which also captures the characteristics of the observed static ME effect. Our proof-of-principle study, demonstrating the control and the optical readout of ME domains in $LiCoPO_4$, lays down the foundation for future ME memory devices based on antiferroelectric-antiferromagnetic insulators.

[1] V. Kocsis *et al.*, arXiv:1711.08124 (2017)

KFM 12.3 Wed 10:00 EB 202

On-off switching of magnetism in ultrathin films of $La_{1-x}Sr_xMnO_3$ gated with an ionic liquid — •Alan Molinari, Robert Kruk, and Horst Hahn — Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344, Eggenstein-Leopoldshafen, Germany

Utilization of electric fields instead of conventional dissipative flowing currents to control magnetism may be the key for the realization of a variety of novel low-power microelectronic devices. In our work we addressed the control of the magnetization of ultrathin (about 3 nm) films of $La_{1-x}Sr_xMnO_3$ (LSMO) by means of ionic liquid (IL) gating. The magnetoelectric (ME) coupling[1,2] at the LSMO/IL interface was investigated under various conditions of temperature and applied voltage via in situ synchronized Superconducting Quantum Interference Device magnetometry and Cyclic Voltammetry. Thanks to the high surface-to-volume ratio of the films and the large amounts of surface charge densities attainable with the IL, ferromagnetism could be reversibly suppressed and restored in LSMO by application of just a few volts. Our results intend to bring to attention some appealing functionalities of solid/liquid ME devices.

[1]A. Molinari et al., Nat. Comm. 8, 15339 (2017), doi:10.1038/ncomms15339

[2]A. Molinari et al., Adv. Mater. 1703908 (2017), doi: 10.1002/adma.201703908

KFM 12.4 Wed 10:15 EB 202

Domain wall engineering as a route towards room temperature multiferroicity — •Konstantin Z. Rushchanskii, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut,

Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Multiferroics are materials that exhibit two or more ferroic order parameters in a single phase. Their room-temperature functionality as well as the strong coupling of magnetic and electric order parameters are desired for devices of future electronics, such as multistate nonvolatile memory cells, electrically controlled spintronic devices, etc. Isostructural $Ga_{0.6}Fe_{1.4}O_3$ (GFO) [1] and ϵ-Fe_2O_3 (eFO) [2] are of special interest, due to simultaneous presence of ferrimagnetic coupling and a polar structure. Recently reported observation of room-temperature mutiferroic behavior in thin films of these compounds made them prospective materials for practical applications. Unfortunately, ferroelectric properties were experimentally observed only for a limited number of samples, and the conditions to have switchable polarization are still unclear.

We employ Density Functional Theory in combination with an evolutionary algorithm [3] to obtain realistic models of polarization switching in eFO and GFO. We will discuss the conditions, under which the films with maximal, switchable remanent ferroelectric polarization are obtained.

We acknowledge the support by GALIMEO Consortium.

[1] A. Thomasson et al., J. Appl. Phys. **113**, 214101 (2013); [2] M. Gich et al., Adv. Mater., **26**, 4645 (2014); [3] http://uspex.stonybrook.edu

15 minutes break

KFM 12.5 Wed 10:45 EB 202

Frustrated magnetism and magnetoelectric switching in RMn2O5 compounds — •Sergey Artyukhin and Louis Ponet — Italian Institute of Technology, Via Morego 30, Genova, Italy

Rare earth manganites RMn2O5 exibit complex magnetism and magnetically induced polarization, with chains of antiferromagnetically coupled Mn ions along a direction geometrically frustrated interchain interactions along b, and the competition of nearest and next-nearest neighbor exchanges along c leading to spiral states in YMn2O5. Here we use Landau theory and model Hamiltonian calculations with parameters obtained from density functional perturbation theory calculations to study magnetoelectric coupling and magnetic switching in these compounds.

KFM 12.6 Wed 11:00 EB 202

A theoretical study on the electronic and magnetic excitation spectra of $BiFeO_3$ by dynamical mean-field theory — •Souvik Paul[1,2], Diana Iusan[1], Patrik Thunström[1], Yaroslav Kvashnin[1], Johan Hellsvik[1,3], Manuel Pereiro[1], Anna Delin[1,3], Biplab Sanyal[1], and Olle Eriksson[1] — [1]Department of Physics and Astronomy, Uppsala University, Sweden — [2]Institute of Theoretical Physics and Astrophysics, Christian-Albrechts-Universität zu Kiel, Germany — [3]Department of Materials and Nano Physics, KTH Royal Institute of Technology, Sweden

Using local density approximation plus dynamical mean-field theory (LDA+DMFT), we have computed the electronic and magnetic excitation spectra of one of the popular multiferroic $BiFeO_3$. Our calculated eletronic spectra match very well with the experimental (hard X-ray photoelectron spectroscopy and resonant photoelectron spectroscopy for the Fe 3*d* states) spectra as compared to the commonly used LDA+U method, which fails drastically to produce the general features of the experimental spectra. This indicates the importance of correctly including the dynamical correlation among the Fe 3*d* orbitals to reproduce the experimental spectroscopic data. The LDA+DMFT derived density of states (DOS) exhibit significant amount of Fe 3*d* states at the position of Bi lone-pairs, implying that the latter are not alone in the spectral scenario. This fact might modify our interpretation about the origin of ferroelectric polarization in this material. Our magnetic excitation spectra computed from the LDA+DMFT results conform well with the inelastic neutron scattering data.

KFM 12.7 Wed 11:15 EB 202

Magnetic field control of cycloidal domains and electric polarization in multiferroic $BiFeO_3$ — •Sándor Bordács[1], Dániel Farkas[1], Jonathan White[2], Robert Cubitt[3], Lisa DeBeer-Schmitt[4], Toshimitsu Ito[5], and István Kézsmárki[1,6] — [1]Department of Physics, Budapest University of Technology and Economics and MTA-BME Lendület Magneto-optical Spectroscopy Research Group, Budapest, Hungary — [2]Laboratory for Neutron Scattering and Imaging, PSI, Villigen, Switzerland — [3]Institut Laue-Langevin, Grenoble, France — [4]Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA — [5]National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, Japan — [6]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany

The magnetic field induced rearrangement of the cycloidal spin structure in ferroelectric monodomain single crystals of the room-temperature multiferroic $BiFeO_3$ is studied using small-angle neutron scattering (SANS). The cycloid propagation vectors are observed to rotate when magnetic fields applied perpendicular to the rhombohedral (polar) axis exceed a pinning threshold value of $\sim$5 T. In light of these experimental results, a phenomenological model is proposed that captures the rearrangement of the cycloidal domains, and we revisit the microscopic origin of the magnetoelectric effect. A new coupling between the magnetic anisotropy and the polarization is proposed that explains the recently discovered magnetoelectric polarization to the rhombohedral axis.

KFM 12.8 Wed 11:30 EB 202

Reversible Modulation of Magnetic Anisotropy in $Pb(Zr_{0.2}Ti_{0.8})O_3$ /$La_{0.8}Sr_{0.2}MnO_3$ Multiferroic Heterostructures — •Anil Rajapitamahuni, Lingling Tao, Evgeny Tsymbal, and Xia Hong — Department of Physics and Astronomy,University of Nebraska-Lincoln, Lincoln,NE, 68588

We report a reversible modulation of in-plane magnetic anisotropy energy (MAE) in 4 nm $La_{0.8}Sr_{0.2}MnO_3$ (LSMO) thin films via ferroelectric field effect induced charge doping facilitated by $Pb(Zr_{0.2}Ti_{0.8})O_3$(PZT) top gate. We employed, planar Hall effect measurements (PHE) to characterize the in-plane magnetic anisotropy in PZT/LSMO heterostructures. The magnetic anisotropy in LSMO is found to be biaxial with easy axes along <110> directions for both polarization states. The extracted biaxial anisotropy fields (H1) from PHE measurements, showed an enhancement in H1 in the accumulation state. Assuming a doping level change of 0.1 electron/Mn due to the polarization switching, the estimated anisotropy energy densities are 0.9 x 10^5 erg/cm^3 and 1.17 x 10^5 erg/cm^3 in the depletion and accumulation states respectively. This corresponds to a 30% enhancement of the MAE in the accumulation state when compared to the depletion state values. First principles density functional theory calculations performed for various Sr doping levels also show an increase in the MAE with an increase in the hole doping, agreeing well with our experimental observations. We attribute this enhancement in MAE to the modification of orbital contribution to spin-orbit coupling via ferroelectric field effect in LSMO.

KFM 12.9 Wed 11:45 EB 202

Magnetoelectric effect in elastic multiferroic composites — •Yuliya Alekhina[1], Liudmila Makarova[1], Tatiana Rusakova[1], Olga Malyshkina[2], and Nikolai Perov[1] — [1]Lomonosov Moscow State University, Moscow, 11999, Russia — [2]Tver State University, Tver, 170100, Russia

Magnetorheological elastomers (MREs) are a type of "smart materials" changing their properties under the influence of external factors. MREs represent magnetic particles distributed in elastic medium. Under the magnetic field magnetic moments of particles tend to align what can lead to their shifting and rotating. Such ordering leads to several effects which can be observed in MREs, e.g. magnetorheological effect. It was previously shown that in MREs with both iron and graphite particles change of electrical resistance can be induced by magnetic field. In this case shifting of magnetic particles under the magnetic field creates the internal stresses in polymer matrix, which lead to displacements of the conductive graphite particles. Similar effect can be observed if ferroelectric particles are added to the MRE [1]. Those internal stresses can affect the movement of ferroelectric particles forcing to or preventing them from shifting and rotation thus changing the polarization process. The reverse effect is also possible: under the electric field, the magnetization process can be changed. Thereby, a type of multiferroic composite with elastically coupled ferromagnetic iron particles and ferroelectic PZT particles was prepared and investigated in this work. The work was financially supported by Grant RFBR 18-32-00354. [1] L.A. Makarova et al., IEEE Transactions on Magnetics, 2017, 53, 11, pp.7

KFM 13: Diamond I

This dedicated focus session represents the production and applications of diamond and diamond related materials in the fields of dielectrics, electronics, high frequency techniques, GHz-THz- applications, mechanics and optics. Also materials/composites like carbides, boron-carbides and nitrides are related materials with excellent mechanical properties. Applications with integrated diamond or related materials in technical systems are part of this session (Nuclear fusion applications,high frequency heating systems and material processing).

Chair: Theo Scherer KIT Karlsruhe

Time: Wednesday 9:30–12:50 Location: E 020

Invited Talk KFM 13.1 Wed 9:30 E 020

Advanced Cell Adhesion of Modified Ultrananocrystalline Diamond Surfaces — •Cyril Popov — Institute of Nanostructure Technologies and Analytics, Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Germany

The interactions of different types of cells with ultrananocrystalline diamond (UNCD) surfaces with H-, O- and NH2-terminations were investigated with respect to cell density and viability. No cyto- or genotoxicity, no adverse effects on the cell viability and physiological responses were detected. The observed fast and strong attachment of the cells was attributed to a favorable combination of topography, surface chemistry and wettability. The enhanced attachment of the neurons was especially advantageous for the immunocytochemical procedures where the cell losses during washing steps were significantly reduced by one order of magnitude. In addition, applying photolithography the integration of a titanium grid structure under the UNCD films allowed for individual assignment of physiologically characterized neurons. The patterning of the UNCD surface termination by a hard mask and two modification steps resulted in guided cell attachment and growth.

KFM 13.2 Wed 10:00 E 020

Quantum Coins and Nano Sensors: Development of Unforgeable Diamond Money — •Alexander Schmidt, Johann Peter Reithmaier, and Cyril Popov — Institute of Nanostructure Technologies and Analytics, Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

The integration of NV centers within diamond nanostructures such as nanopillars and AFM tips can be used for the development of quantum coins implementation and quantum sensing of magnetic fields at a nanoscale. Here we report on our two main fabrication procedures for structuring of nanocrystalline diamond (NCD) films: First, for highly dense arrays of nanopillars and second for AFM tips. The fabrication process of nanopillars consisted of their definition by electron beam lithography (EBL) applying a hard mask and subsequent inductively coupled plasma reactive ion etching (ICP RIE) with oxygen. The lateral distances of the pillar arrays with 200, 100 and 50 nm diameter were decreased up to the highest package density achieveable. NCD AFM tips were fabricated by means of the moulding technique, using conventional photolithography and anisotropic wet etching of the silicon substrate.

KFM 13.3 Wed 10:20 E 020

Application of UNCD Layers as Implant Coatings — •Daniel Merker[1], Silviya Stateva[2], Rolf Merz[3], Michael Kopnarski[3], Johann Peter Reithmeier[1], Margarita Apostolova[2], and Cyril Popov[1] — [1]Institut für Nanostrukturtechnologie und Analytik, Kassel, Germany — [2]Roumen Tsanev Institute of Molecular Biology, Sofia, Bulgaria — [3]Institut für Oberflächen- und Schichtanalytik GmbH, Kaiserslautern, Germany

Due to the excellent mechanical properties combined with good biocompatibility thin diamond layers are considered as a promising material for biomedical applications like implant coatings. We performed tribological measurements of ultrananocrystalline diamond (UNCD) coated titanium samples against steel and diamond counterparts to investigate their friction behavior. The key property of an implant coating is the interaction with the surrounding tissue to prevent inflammatory responses but on the other hand to promote the integration of the implant into the tissue. We prepared UNCD samples with and without plasma modification of the surface and used three different cell lines related to the generation of new blood vessels and bone matter to study the effects of the different surfaces on the cell adhesion by immunostaining studies and the protein content of the cells by bioinformatic analysis of the proteome. Additionally, we aim to provide the coating with antimicrobial ability by embedding silver nanoparticles into the coating that release silver ions which are known as effective antibacterial agents.

KFM 13.4 Wed 10:40 E 020

Magnetic Resonance in Defect Spins via Spin Waves — •Clara Mühlherr, Vladyslav Shkolnykov, and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

Searching for quantum systems to realize quantum computation, the nitrogen-vacancy (NV) center in diamond has been intensively studied for years. Despite favorable properties such as remarkable coherence times, an application of ensembles of NV centers to perform quantum computing raises some technical issues. Since a direct coupling of NV centers via spin-spin dipolar interaction requires the NV centers to be separated by less than a few nanometers, this proximity limits the addressability of a single center. To overcome this problem, enhancement of coherent interaction between NV centers and a microwave field recently has been demonstrated using spin waves propagating in an yttrium iron garnet (YIG) film [1]. We analyze the optically detected magnetic resonance (ODMR) spectra by combining the occurring resonances and the orientation of the external magnetic field in the YIG. In that way, the crystal orientation of the NV centers is identified, which, in turn, nicely links to applications of NV centers for sensing. In order to explain the coupling mechanism and to estimate the enhancement of the coupling strength, we theoretically calculate the amplitude of the spin waves in the YIG.

[1] P. Andrich *et al.* Long-range spin wave mediated control of defect qubits in nanodiamonds. *npj Quantum Information* **3**, 28 (2017).

20 min. break

Invited Talk KFM 13.5 Wed 11:20 E 020

CVD diamond for high power electronic devices — •Verena Zürbig — Fraunhofer-Institut für Angewandte Festkörperphysik IAF, Freiburg, Germany

CVD single-crystalline diamond is a promising wide band gap semiconductor for the fabrication of high power, high frequency and high temperature electronic devices due to its outstanding physical properties such as high breakdown electric field, high thermal conductivity and high electron and hole mobilities. Diamond high power devices have been intensively investigated for several years and are a promising alternative to SiC- and GaN-based high power electronic devices. The realization of uni- and bipolar devices requires the ability to grow high quality phosphorous- and boron-doped single-crystalline diamond layers on (100) and (111) oriented crystals along with the ability of 3D-technology to manufacture high power electronic devices. In this talk, a detailed presentation of phosphorous- and boron-doped diamond layer-growths regarding their crystalline quality and its influence on electronic properties will be given. In addition, recently diamond-based power electronic devices will be summarized.

KFM 13.6 Wed 11:50 E 020

Electrical characterization of diamond-based Schottky-diodes for high power electronics — •Lucas Pinti[1], Philipp Reinke[1], Fouad Benkhelifa[1], Lutz Kirste[1], Christian Giese[1], Tobias Erlbacher[2], Andreas Schletz[2], Volker Cimalla[1], Christoph E. Nebel[1], Oliver Ambacher[3], and Verena Zuerbig[1] — [1]Fraunhofer IAF, Freiburg, Germany — [2]Fraunhofer IISB, Erlangen,

Germany — [3]INATECH, Freiburg, Germany

In power electronics, the enhancement of energy efficiency and reduction of module volume are major points for innovative voltage converter system. Switching and conduction losses in common Si-based power electronic devices and the consequential need of cooling systems to guarantee reliable operation of such systems reduce the overall efficiency and therefore represent additional costs. Diamond as a new wide-band-gap semiconductor material is a promising extension in terms of voltage and heat dissipation in comparison to Si-based power electronic devices. With its outstanding physical properties like high breakdown electric field, high carrier mobilities and high thermal conductivity diamond has the best requirements to enable semiconductor power devices with low losses and minimized cooling efforts. In our presentation, we will report on the electrical characterization of vertical single-crystalline diamond Schottky diodes, which are fabricated by a CVD process. Temperature dependent IV characteristics as well as a detailed analysis of important device parameters like blocking voltage and specific on-resistance of the diodes will be given and compared to state of the art power diodes suitable for power converter modules.

KFM 13.7 Wed 12:10 E 020

Messverfahren zur Bestimmung der Wärmeleitfähigkeit an dünnen Diamantschichten an Hand von Beispielen — •Mario Bähr, Indira Käpplinger, Alexander Lawerenz und Thomas Ortlepp — CiS Forschungsinstitut für Mikrosensorik GmbH, Konrad-Zuse-Str. 14, 99099 Erfurt, Germany

Diamant besitzt in seiner einkristallinen Form einen der höchsten Wärmeleitfähigkeitskoeffizienten (>2000 W/mK). Diese wird nur bei Diamant gepaart mit einem über mehrere Größenordnungen einstellbaren elektrischen Widerstand von 10^4-10^{14} Ohmcm. Daher ist eine technische Nutzung von höchstem Interesse im Bereich der Aufbau- und Verbindungstechnologie temperaturkritischer Bauelemente, die einem effektiven Wärmemanagement bedürfen. Diese sind bspw. Leuchtdioden oder (opto-) elektronische Hochleistungsbauelemente. Kosteneffizient könnten Diamantschichten als Wärmespreizer auch als dünne Schichten mit Dicken von <50 um eingesetzt werden. Dazu wird die Diamantschicht auf einem Träger (=Wärmesenke) synthetisiert und strukturiert. Dieser Ansatz wurde verfolgt und Siliziumträger mit einer wärmespreizenden synthetischen Diamantschicht simuliert, hergestellt und mit verschiedenen Verfahren charakterisiert. Besonderes Augenmerk liegt auf der Bestimmung der Wärmeleitfähigkeit der dünnen Diamantschichten. Gegenübergestellt werden die 3-Omega-Methode angewendet an unterschiedlichen Probenkonfigurationen und das Laser-Flash-Verfahren in verschiedenen Konfigurationen. Da für die Anwendung relevant, wird auf die Unterscheidung der transversalen und der lateralen Wärmeleitfähigkeit hingearbeitet.

KFM 13.8 Wed 12:30 E 020

Holonomic Quantum Control of the state of an NV-center in Diamond — •Vlad Shkolnikov[1], Brian Zhou[2], Paul Jerger[2], Joseph Heremans[2,3], Guido Burkard[1], and David Awschalom[2,3] — [1]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [2]Institute for Molecular Engineering, University of Chicago, Chicago, Illinois 60637, USA — [3]Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA

Geometric phases arising from cyclic evolution of quantum systems open new strategies for constructing robust quantum technologies. Here, we demonstrate arbitrary single qubit holonomic gates from a single cycle of nonadiabatic evolution of the electron spin of an NV-center [1]. Our method varies the amplitude, phase, and detuning of a two-tone optical field to gain full control over the state of the qubit with arbitrary rotation axes and angles. We analyze the robustness of detuned gates using the Lindblad formalism and show the gate fidelity to be mostly defined by the lifetime of the excited state of the NV. We experimentally and theoretically prove that single cycle gates are better than those consisting of two concatenated cycles.

[1] Brian B. Zhou, Paul C. Jerger, V.O. Shkolnikov, F. Joseph Heremans, Guido Burkard, and David D. Awschalom Phys. Rev. Lett. 119, 140503

KFM 14: Materials for Energy Storage I (joint session KFM/CPP)

Organizer: Martin Diestelhorst - Martin-Luther-Universität Halle-Wittenberg - Halle

Time: Wednesday 9:30–12:30 Location: EMH 025

Invited Talk KFM 14.1 Wed 9:30 EMH 025

Resource-efficient dielectric materials for short-time energy storage — •Stephan Krohns — Experimental Physics V, University of Augsburg, 86159 Augsburg

Materials exhibiting so-called colossal effects have an enormous potential for future use in correlated electronics, including capacitors for energy storage. The search for functional dielectrics showing colossal dielectric constants (CDC) is still an active field of research [1].

Beside the pure materials properties, also the scarcity and possible future shortages of used key elements in this modern technology is in the focus of scientific interest. An imminent challenge of modern materials science is the development of materials with less critical elements that have comparable or better functionalities than those currently used.

In this talk, I address the pure materials science perspective focusing on the research of CDC materials like crystals showing barrier layer capacitances [2] as well as ionic liquids. The latter are promising candidates for electrolytes used in supercapacitors [3]. Furthermore, I present a practical guideline for basic research implementing resource strategy aspects [4] as well as a possible scenario for the system and market integration of those short-term energy storages [5].

[1] S. Krohns et al., Nat. Mat. 10, 899 (2011).
[2] E. Ruff et al., Phys. Rev. Lett. 118, 036803 (2017).
[3] P. Sippel et al., Sci. Rep. 5, 13922 (2015).
[4] Ch. Helbig et al., Sust. Mat. & Techn. 12, 1 (2017).
[5] M. Hassler et al., OR Spectrum 38, 633 (2016).

KFM 14.2 Wed 10:00 EMH 025

Dielectric properties of ionic liquid based electrolytes for future energy-storage systems — •Pit Sippel and Stephan Krohns — Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany

Electrolytes are essential for energy storage systems like electric double layer capacitor (EDLC). The so-called electrode polarization is the driving mechanism for energy storage in EDLCs. To enhance the properties of EDLCs, potential new electrolytes are investigated by various methods. Dielectric spectroscopy is a powerful tool analyzing the electric properties of liquids. This technique allows measuring the relaxation times of dynamic processes and ionic conductivity in a broad frequency and temperature range. Especially, the ionic conductivity is an essential figure of merit for any energy-storage application. This talk addresses the dielectric properties of ion conducting liquids with special emphasize put on ionic liquids (ILs). The revealed spectra are analyzed using equivalent circuits, which enable investigating the important electrode polarization effect. ILs offer outstanding properties (e.g., low volatility and high electrochemical stability) making them promising candidates for solvent-free electrolytes, which may improve energy-storage systems. However, the applicability of ILs is still hampered due to their rather low conductivity. We address the question if this conductivity can be optimized by mixing pure ILs taking into account the non-canonical super-Arrhenius temperature dependence [1].
[1] E. Thoms *et al.*, Sci. Rep. **7**, 7463 (2017).

KFM 14.3 Wed 10:20 EMH 025

Influence of the glass-ceramic synthesis route on the ionic conductivity of the sodium solid electrolyte Na_2O-Y_2O_3-SiO_2 — •Wolfram Münchgesang[1], Dörthe Wagner[2], Mykhaylo Motylenko[3], Jochen Schilm[2], David Rafaja[3], and Dirk C. Meyer[1] — [1]Institut für Experimentelle Physik, Technische Universität Bergakademie Freiberg, 09599 Freiberg, Germany — [2]Fraunhofer-Institut für Keramische Technologien und Systeme IKTS, 01277 Dresden, Germany — [3]Institut für Werkstoffwissenschaft, Technische Universität Bergakademie Freiberg, 09596 Freiberg, Germany

The development of room-temperature solid electrolytes (SEs) is one of the keys for the realization of solid-state batteries – a post lithium-ion

technology, with probably better performance than this. For SEs, a glass-ceramic synthesis route (GCSR) is particularly suitable, because this is less expensive than other production methods and can be used on an industrial scale.

The maximum achievable conductivity (C) of SEs is determined by the used ionic-conductive phase (ICP), which is crystalline $Na_5YSi_4O_{12}$ in our case. In practice C is strongly influenced by the microstructure of the SE, in particular by the formation of a suitable percolation path; which is determined by the ratio of the ICP and its crosslinking. We will present the influence of different GCSRs on the microstructure of the SE and the resulting conductivity change.

This work was financed by the Federal Ministry (FM) of Education and Research within the project SyNeSteSia (05K14OFA) and the FM for Economic Affairs and Energy within the project BaSta (0325563).

KFM 14.4 Wed 10:40 EMH 025

Water Adsorption on a n-Si/NiO Photoanode - Cryo Photoelectron Spectroscopy in the Frozen Electrolyte Approach — •Mathias Fingerle, Sven Tengeler, Wolfram Calvet, Thomas Mayer, and Wolfram Jaegermann — Surface Science Division, Department of Materials Science, Technical University Darmstadt, Otto-Berndt-Str. 3, D-64287 Darmstadt, Germany

In the course of the BMBF InnoEMat project Fundamentals of Electrochemical Interfaces: Semiconductor/Electrolyte, elemental charge transfer processes at solid/liquid interfaces are studied via cryo photoelectron spectroscopy and post-operando experiments. Here, the interaction of water with a magnetron-sputtered nickel oxide thin film on an n-type silicon photo-anode is investigated in perspective to oxygen evolution. The substrate was exposed in-situ stepwise to gas phase water up to 10 L at liquid N2 temperature and analyzed via X-ray and UV photoelectron spectroscopy in the so called frozen electrolyte approach. Photoemission of the pristine NiOx layer shows the presence of stoichiometric NiO and Ni2O3 as well as of non-stoichiometric phases. In the monolayer range, molecular and dissociative adsorption is detected assigned to the NiO respective Ni2O3 phase. Initially, the emissions of the molecular adsorbed water species interacting with NiO are found at 0.8 eV lower binding energies as compared to water related emissions for higher coverages with binding energies commonly assigned to H2O-H2O interaction. In addition to the chemical analysis, the electronic structure of the n-Si/SiOx/NiOx/H2O photoanode is measured and discussed.

20 min. break

KFM 14.5 Wed 11:20 EMH 025

Morphologischer Einfluss von BaTiO3 Partikeln auf die Leitfähigkeit und Speicherzeit von Oxid*Polymer-Filmkondensatoren — •Sandra Wickert[1], Till Mälzer[2], Frank Apsel[3], Tino Band[4], Hartmut Leipner[5], Martin Diestelhorst[6] und Stefan Ebbinghaus[7] — [1]enfas GmbH, D-80809 — [2]enfas GmbH, D-80809 — [3]enfas GmbH, D-80809 — [4]Institut für Physik, MLU Halle-Wittenberg, D6120 — [5]IZM, MLU Halle-Wittenberg, D6120 — [6]Institut für Physik, MLU Halle-Wittenberg, D6120 — [7]Institut für Chemie, MLU Halle-Wittenberg, D6120

Der Einfluss der Morphologie von BaTiO3 Partikeln auf die Leitfähigkeit und die daraus resultierende Speicherzeit von BaTiO3/P(VDF-HFP)-Folienkondensatoren wurde untersucht. Dazu wurden über die Mischoxidsyntheseroute BaTiO3*Partikel unterschiedlicher Form und Größe hergestellt und in Lösungen des ferroelektrischen Polymers P(VDF-HFP) suspendiert. Über eine Rakelanlage wurden diese Lösungen in Folien gegossen und nach verschiedenen Verfahren getrocknet. Nach Kontaktierung erfolgte die dielektrische Auswertung der so erhaltenen Kondensatoren mittels unipolarer zyklischer Polarisationsmessungen. Es konnte gezeigt werden, dass sowohl die Größe als auch die Form der BaTiO3-Partikel eine entscheidende Rolle für die Gesamtleitfähigkeit des Systems spielen. Außerdem konnte das bisherige core-shell-Modell für die Bildung von BaTiO3 erweitert werden, so dass nicht nur die Entstehung der Einzelpartikel beschrieben wird, sondern auch die Bildung von Agglomeratstrukturen erklärt werden kann.

KFM 14.6 Wed 11:40 EMH 025

Investigation of electrical conductivity and dielectric properties in ceramic-polymer composite films — •Till Mälzer[1,4], Tino Band[2], Sandra Wickert[3,5], Frank Apsel[1,5], Hartmut S. Leipner[1], Martin Diestelhorst[2], and Stefan Ebbinghaus[3] — [1]Center of Materials Science, Martin-Luther-University Halle-Wittenberg (MLU), 06120 Halle (Saale) — [2]Department of Physics, MLU — [3]Department of Chemistry, MLU — [4]enfas GmbH, 86668 Karlshuld — [5]enspring GmbH, 06120 Halle (Saale)

Dielectric materials with high energy storage density are of great importance for power electronics. Ceramic-polymer composites have been evaluated as a candidate for dielectric materials for new-type capacitors, due to the possibility to tailor materials properties by proper design for specific applications. Besides dielectric properties in majority of studies, the electrical conduction of the ceramic-polymer composite films has been disregarded. We report on results of composite films consisting of the two ferroelectric materials P(VDF-HFP) as polymer matrix and BaTiO3 as filler, each known for its high permittivity in its particular material class. Composite films with different size and concentration of BaTiO3 particles were fabricated via a solution cast doctor blade method. We studied the influence of particle size, agglomeration, particle distribution and filler concentration on electrical conductivity and the dielectric properties energy density, permittivity and breakdown strength of the composite films. We used charge-voltage measurements for dielectric investigations and for morphological studies X-ray diffraction and scanning electron microscopy.

Invited Talk KFM 14.7 Wed 12:00 EMH 025

Dielectric Polymer Nanocomposites for Electrical Energy Storage — •Qing Wang — The Pennsylvania State University

The demand for high-performance dielectric materials arises from numerous emerging energy storage and conditioning applications such as electric vehicles, wind generators, solar converters, and aerospace power systems. This talk will describe our most recent efforts to develop the dielectric polymer nanocomposites for capacitive energy storage applications. Specifically, the introduction of boron nitride nanosheets (BNNSs) into the polymers yields significantly reduced high-field loss and improved thermal conductivity, giving rise to great improvements in the charge-discharged efficiency and discharged energy density at high temperatures. The sandwich-structured composites with BNNSs spreading throughout the outer polymeric layers and high-dielectric-constant nanoparticles in the interior layer has been designed and experimentally demonstrated. More recently, chemical-vapor-deposited hexagonal boron nitride (h-BN) has been coated onto the surface of the polymer films. The h-BN-coated polymer films are capable of operating with >90% efficiencies and delivering high energy densities even at a temperature close to the glass transition temperature of polymer. Challenges along with future research opportunities will also be discussed.

KFM 15: Multiferroic Oxide Thin Films and Heterostructures I (joint session KFM/TT/MA)

Organizers: César Magén - University of Zaragoza, Aragón (Spain); Kathrin Dörr - Martin-Luther-Universität Halle-Wittenberg - Halle

Multiferroic oxide thin films and magnetoelectrically coupled oxide heterostructures are among the most attractive topics in the field of Complex Oxides. Within this extensive family of compounds, which are characterized by an unprecedented wealth of physical phenomena upon subtle variations of the structure or chemistry, multiferroics stand out due to the exciting novel physics underlying the coexistence and coupling of multiple ferroic orders. This exotic behavior bestows inherent multifunctionality upon these systems (either single-phase or heterostructure multiferroics), providing strong potential for future nanoelectronic devices.

Time: Wednesday 9:30–12:45 Location: EMH 225

Invited Talk KFM 15.1 Wed 9:30 EMH 225

Oxygen vacancy controlled functionalities at interfaces of multiferroic tunnel junctions. — •Jacobo Santamaria — GFMC. Universidad Complutense 28040 Madrid

Oxygen vacancies are the most common defect in oxide perovskite oxides. Important applications are associated to their controlled generation and transport in electrochemical energy (fuel cells and batteries) and memory (memristors) devices. At interfaces oxygen vacancies can accumulate under the action of external electric fields and, especially in nanostructures be the source of novel, yet unreported, functionalities. Here we demonstrate the dynamic control of the vacancy profile in the nanometer thick barrier of a ferroelectric tunnel junction. Oxygen vacancies generated at an electrochemically active electrode accumulate towards the asymmetric interfaces of a ferroelectric tunnel barrier under the action of an external electric field and their ensuing doping effect modify the stability of ferroelectric polarization. I will further show that oxygen vacancies in a ferroelectric tunnel barrier may stabilize unexpected domain structures which control the tunneling transport providing a major step forward towards the new concept *The Wall is the Device* , to exploit the electronic properties of domain walls for ferroelectric tunnel barriers with new functionalities.

KFM 15.2 Wed 10:00 EMH 225

Structure and Magnetism of the Co/PZT/LSMO Interface — •Holger Meyerheim[1], Arthur Ernst[2], Katayoon Mohseni[1], Andrey Polyakov[1], Nathalie Jedrecy[3], Andy Quindeau[1], Victor Antonov[1], Manuel Valvidares[4], Hari Vasili[4], and Pierluigi Gargiani[4] — [1]MPI f. Mikrostrukturphysik, D-06120 Halle — [2]Inst. für Th. Physik, JKU, A-4040 Linz, Austria — [3]INSP, UPMC-Sorbonne Univ., 75005 Paris, France — [4]Alba, 08290 Cerdanyola del Vallés, Spain

Using surface x-ray diffraction, x-ray absorption fine structure and x-ray circular dichroism (XMCD) experiments we have studied the geometric and magnetic properties of the Co/Pb($Ti_{0.8}Zr_{0.2}$)O_3 interface. Co deposition in submonolayer amounts on the 2 unit cells thick (Ti,Zr)O_2 terminated Pb ($Ti_{0.8}Zr_{0.2}$)O_3 (PZT) layer leads to the formation of a perovskite type structure with Co-O distances of approximately 2.0 Å (octahedral) and 2.8 Å (cubic) in addition to a metallic Co-Co correlation near 2.4 Å. Co-$L_{2,3}$-XMCD spectra also reveal different Co environments, especially two Co-O contributions (A) and (B) related to the octahedral coordination (m=2.69μ_B) and the cubic coordination (m=2.33 μ_B). The XMCD analysis also evidences an anti-FM oriented induced moment at the PZT top layer Ti site (m=-0.005μ_B) related to the negative tunneling electro resistance effect. This result supports the "hybridization model" suggested by D.Pantel et al., Nat. Mat. 11, 289 (2012).
Support by SFB 762 (TP A5) is acknowledged. We thank E. Fonda (Samba at Soleil) and the ALBA staff for help during the experiments.

KFM 15.3 Wed 10:15 EMH 225

Interfacial mechanisms in magneto-electric bismuth iron garnet thin films — •Laura Bocher[1], Adrien Teurtrie[1,2], Elena Popova[2], Odile Stéphan[1], Alexandre Gloter[1], and Niels Keller[2] — [1]Laboratoire de Physique des Solides - UMR 8502 CNRS, Université Paris-Sud, Orsay, FR — [2]Groupe d'Etude de la Matière Condensée - UMR8635 CNRS, UVSQ, Université Paris-Saclay, FR

Bismuth iron garnet (BIG) is ferrimagnetic with a relatively high magnetization (1600 G at 300 K), a magnetic ordering temperature from 650 K, and a giant Faraday rotation [1]. More recently, we evidenced a strong magneto-electric coupling at 300 K and above in BIG thin films opening new perspectives for an electric control of the magnetization [2]. However BIG can solely be elaborated in thin film form using non-equilibrium growth techniques and no bulk reference exists for conventional investigations. Hence precise knowledge on the atomic and electronic structures of BIG thin films remains a key challenge to understand better their structure-property relationships.

Here we will shed light on BIG thin films using advanced electron spectro-microscopy techniques, i.e. Cs-STEM/EELS, to identify how its cubic structure can accommodate locally different lattice mismatches through a variety of relaxation mechanisms and verify down to the scale of the atomic columns any possible cation interdiffusion and/or electronic reconstruction at the film/substrate interface [3].

[1] M. Deb, et al. J. Phys. D 45 (2012) 455001. [2] E. Popova et al. APL 110 (2017) 142404. [3] E. Popova et al. JAP 121 (2017) 115304

KFM 15.4 Wed 10:30 EMH 225

Nonlinear spin-lattice coupling in EuTiO3: novel two-dimensional magneto-optical device for light modulation — •Annette Bussmann-Holder[1], Krystian Rolder[2], and Jürgen Köhler[1] — [1]Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [2]2Institute of Physics, University of Silesia, ul. Uniwersytecka 4, 40-007 Katowice, Poland

EuTiO3 is antiferromagnetic at low temperature, namely below TN=5.7K. In the high temperature paramagnetic phase the strongly nonlinear coupling between the lattice and the nominally silent Eu 4f7 spins induces magnetic correlations which become apparent in muon spin rotation experiments and more recently in birefringence measurements in an external magnetic field. It is shown here, that high quality films of insulating EuTiO3 deposited on a thin SrTiO3 substrate are versatile tools for light modulation. The operating temperature is close to room temperature and admits multiple device engineering. By using small magnetic fields birefringence of the samples can be switched off and on. Similarly, rotation of the sample in the field can modify its birefringence Δn. In addition, Δn can be increased by a factor of 4 in very modest fields with simultaneously enhancing the operating temperature by almost 100K. The results can be understood in terms of paramagnon phonon interaction where spin activity is achieved via the local spin-phonon double-well potential.

KFM 15.5 Wed 10:45 EMH 225

Complexity in the structural and magnetic properties of almost multiferroic EuTiO3 thin films — Zurab Guguchia[1], Zaher Salman[2], •Hugo Keller[3], Krystian Roleder[4], Jürgen Köhler[5], and Annette Bussmann-Holder[5] — [1]Department of Physics, Columbia University, New York, New York 10027, USA — [2]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — [3]Physik-Institut der Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland — [4]Institute of Physics, University of Silesia, ul. Uniwersytecka 4, PL-40-007 Katowice, Poland — [5]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

In a number of recent publications hidden magnetic properties at high temperatures have been reported for EuTiO3 (ETO), which orders antiferromagnetically below TN=5.7K. In addition, structural phase transitions have been discovered which correlate with the magnetic responses and can be tuned by a magnetic field. In order to identify the magnetic properties of ETO at temperatures well above TN, low-energy muon-spin rotation (μSR) experiments have been performed on thin films of ETO which exhibit all properties observed in bulk materials and are thus well suited to conclude about the magnetic order

of the bulk. The μSR data reveal anomalies at 282 and 200 K related to the structural phase transitions in accordance with birefringence results. In addition, a transition to some kind of magnetic order below 100 K was observed as previously indirectly deduced from conductivity and dielectric constant measurements.

KFM 15.6 Wed 11:00 EMH 225

Surface reconstructions and related local properties of a $BiFeO_3$ thin film — •Pengxiang Xu[1] and Lei Jin[2] — [1]Institute for Theoretical Physics, ETH Zurich — [2]Peter Grünberg Institute (PGI-5), Forschungszentrum Juelich

Coupling between lattice and order parameters, such as polarization in ferroelectrics and/or polarity in polar structures, has a strong impact on surface relaxation and reconstruction. However, up to now, surface structures that involve the termination of both matrix polarization and polar atomic planes have received little attention, particularly on the atomic scale. Here, we study surface structures on a $BiFeO_3$ thin film using atomic-resolution scanning transmission electron microscopy and spectroscopy. Two types of surface structure are found, depending on the polarisation of the underlying ferroelectric domain. On domains that have an upward polarisation component, a layer with an Aurivillius-Bi_2O_2-like structural unit is observed. Dramatic changes in local properties are measured directly below the surface layer. On domains that have a downward polarisation component, no reconstructions are visible. Calculations based on ab initio density functional theory reproduce the results and are used to interpret the formation of the surface structures.

15 min. break

KFM 15.7 Wed 11:30 EMH 225

Domain engineering in BFO films — •Yeseul Yun[1,2], Niranjan Ramakrishnegowda[1,2], David Knoche[1,2], Daesung Park[1,2], and Akash Bhatnagar[1,2] — [1]Zentrum für Innovationskompetenz SiLi-nano, Halle (Saale), Germany — [2]Martin Luther Universität Halle-Wittenberg, Halle (Saale, Germany)

Multiferroic materials have attracted great attention due to their unusual physical properties and potential in device applications. The lead-free bismuth ferrite ($BiFeO_3$) is one of the most promising candidates. The domain structure plays a crucial role in determining ferroelectric and magnetic properties. Domains and domain walls can be modulated by parameters such as epitaxial strain, film thickness, substrate termination and presence of conductive layers.

In this study, we investigate the role of plume-related characteristics in obtaining long range order of ferroelastic domains in $BiFeO_3$ films. BFO/LSMO hetero-structures were fabricated using PLD on STO (001) substrate with different O_2 partial pressures. Preferential nucleation and long range ordering of 71° domain walls was achieved by varying the plume density, indicating the importance of plasma plume dynamics for the evolution of domain structure in the films. The role of strain and electrostatic energies was also analyzed in conjunction. The thickness of BFO was varied to modulate the extent of strain, while the electrostatic conditions were tuned by the thickness of LSMO.

KFM 15.8 Wed 11:45 EMH 225

Domain Engineering of the Bulk Photovoltaic Effect in Bismuth Ferrite — •David Knoche[1,2], Niranjan Ramakrishnegowda[1,2], Yeseul Yun[1,2], and Akash Bhatnagar[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany — [2]Zentrum für Innovationskompetenz SiLi-nano, Halle (Saale), Germany

The photovoltaic (PV) effect in multiferroic bismuth ferrite (BFO) can be largely attributed to the bulk photovoltaic (BPV) mechanism. The mechanism is associated to the absence of inversion symmetry in these materials. The principle of the BPV effect, that results in an above-bandgap open circuit voltage (V_{oc}), differs from the well-known photovoltaic effect observed in semiconductors like silicon, and still demands in-depth analysis. In this regard, the contribution of ferroic aspects, such as orientation of domains, is crucial and can be potentially used as a tuning parameter.

Thin films of single crystalline $BiFeO_3$ were grown epitaxially via pulsed laser deposition. Planar electrodes with different in-between distances were deposited on top of the sample. The domain orientations within the measurement gap were manipulated by applying high electric fields across the electrodes. Gradual increment in the applied electric field was crucial in obtaining intermediate domain architectures, that were visualized with piezo force microscope (PFM). Photoelectrical response was measured in conjunction to evaluate the influence on Voc and short circuit current.

KFM 15.9 Wed 12:00 EMH 225

Investigation of a-domain formation in Pb(Zr,Ti)O3 thin films — •Niranjan Ramakrishnegowda[1,2], Yeseul Yun[1,2], Daesung Park[1,2], and Akash Bhatnagar[1,2] — [1]Zentrum für Innovationskompetenz SiLi-nano, Halle (Saale), Germany — [2]Martin Luther Universität Halle-Wittenberg, Halle (Saale), Germany

Strain engineering of ferroelectric/ferroelastic domains is an active area of research nowadays, as it provides an exotic pathway to tune the resultant properties of ferroic materials. Since the domains can be also ferroelastic, the extent of strain, applied via the substrate-film lattice parameter mismatch, can be used to define the domain width, orientation and position. However, the persistence of the strain across the thickness of the film is largely affected by growth related process parameters.

In the case of $Pb(Zr,Ti)O_3$, one of the most widely investigated ferroelectric, recent studies involving asymmetric substrates allowed to fine tune the nucleation of a-domains, and the associated domain wall thickness. The proposed prerequisite condition of $a_{film} < a_{substrate} < c_{film}$ was satisfied. In this work we attempt to further analyze this condition by growing PZT films on symmetric $SrTiO_3$ substrates. The role of depolarization field was evaluated by the use of conductive oxide layers sandwiched between the film and the substrate. The usually neglected contribution of target density and purity will be also elaborated.

KFM 15.10 Wed 12:15 EMH 225

Continuous control of morphotropic phases by strain doping — •Andreas Herklotz[1], Stefania Florina Rus[2], Er-Jia Guo[3], Kathrin Dörr[1], and Thomas Zac Ward[3] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania — [3]Oak Ridge National Laboratory, Oak Ridge, USA

The realization of a strain-driven morphotropic phase boundary in epitaxial $BiFeO_3$ (BFO) films has broadened this definition to single-phase materials and opened up great potential for advanced applications. However, a greater success of morphotropic systems in thin film technologies would require a *ex situ* control of the thin film's composition or strain state that is practically impossible with standard epitaxy approaches. Here we demonstrate that *ex situ* strain doping via low-energy helium implantation induces a complete phase transition from epitaxial rhombohedral-like to supertetragonal BFO films. This control over morphotropic phases is highly tunable and fully reversible via a high temperature anneal. We argue that strain doping of morphotropic films creates a new phase space based on internal and external lattice stress that can be seen as an analogue to temperature-composition phase diagrams of classical morphotropic ferroelectric systems.

This effort was wholly supported by the US Department of Energy (DOE), Office of Basic Energy Sciences (BES), Materials Sciences and Engineering Division, with user projects supported at ORNLs Center for Nanophase Materials Research (CNMS).

KFM 15.11 Wed 12:30 EMH 225

Mechanical reading of ferroelectric polarity — •Gustau Catalan[1], Kumara Cordero[2], and Neus Domingo[2] — [1]ICREA-Institucio Catalana de Recerca i Estudis Avançats, Barcelona, Catalunya — [2]ICN2-Institut Catala de Nanociencia i Nanotecnologia, Barcelona, Catalunya

Flexoelectricity is polarization induced by strain gradient. It is closely related to piezoelectricity (polarization induced by strain), a phenomenon for which it was originally viewed as potential substitute. More recently, however, it has become apparent that very exciting new functionalities can be achieved when we combine both flexoelectricity and piezoelectricity in ferroelectrics.

One such functionality, reported in 2012, was the seminal discovery that strain gradients induced by the tip of an atomic force microscope (AFM) could mechanically *write* ferroelectric domains without applying any voltage. Here, we would like to report the complementary effect: the combination of flexoelectricity and piezoelectricity allows *reading* the polar sign of ferroelectric domains from pure (voltage-free) mechanical response.

KFM 16: Lithography I: Focused Electron Beam Induced Processing: 3D Nano-Printing for Material Science (Focussed Session): Morning Session (joint session DS/KFM)

Considering 3D printing using fused-deposition modeling or higher-resolution variants with lasers applicable to polymers and metals, an analogous approach exists on the nanometer scale. With the aid of focused electron beam-induced deposition (FEBID) it is possible to create solid-state structures on the nanoscale. However, in contradistinction to large-scale 3D printing of simple plastic or metallic structures, FEBID is able to directly provide nano-materials with a wealth of interesting electronic, optical and magnetic properties. Due to this, focused electron beam-induced deposition has experienced a rapid expansion in the breadth of its application fields over the last 10 years. FEBID uses precursor gases which, being adsorbed on a surface, are dissociated in the focussed electron beam to form the deposit. Intensive research has pushed the capabilities of FEBID in two important areas. It is now possible to obtain fully metallic nanostructures of Fe, Co and FeCo-alloys and also of Au and Pt. In addition, very recently the simulation-guided nano-manufacturing of 3D structures has matured to such a degree that even complex 3D objects can now be fabricated under controlled conditions. The focused session will address these new developments spanning the range from the fundamentals of electron-precursor interaction, covering aspects of the rational design of optimized precursors, and showing recent work on superconducting, magnetic and plasmonically active materials, both in 2D and 3D.

Organized by

Name: Prof. Dr. Michael Huth, Institution: Physikalisches Institut, Goethe-Universität, City: Frankfurt am Main, Country: Germany, Email: michael.huth@physik.uni-frankfurt.de, Telephone number: +49-69-798-47235

Name: Ass. Prof. Dr. Harald Plank, Institution: Institut für Elektronenmikroskopie und Nanoanalytik, TU Graz, City: Graz, Country: Austria, Email: harald.plank@felmi-zfe.at, Telephone number: +43-316-873-8821

Name: Dr. Ivo Utke, Institution: EMPA, Swiss Laboratories for Materials Science and Technology, City: Thun, Country: Switzerland, Email: Ivo.Utke@empa.ch, Telephone number: +41-58-765-6257

Time: Wednesday 9:30–13:00 Location: H 2032

Invited Talk KFM 16.1 Wed 9:30 H 2032

3D direct-write nanofabrication using an electron beam — •Jason Fowlkes[1], Robert Winkler[2,3], Eva Mutunga[4], Brett Lewis[5], Harald Plank[2,3], and Philip Rack[5] — [1]Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — [2]Institute for Electron Microscopy and Nanoanalysis, Graz University of Technology, 8010 Graz, Austria — [3]Graz Centre for Electron Microscopy, 8010 Graz, Austria — [4]Bredesen Center for Interdisciplinary Research, The University of Tennessee, Knoxville, 37996, USA — [5]Department of Materials Science and Engineering, The University of Tennessee, Knoxville, 37996, USA

The deposition of 3D nanomaterials with precise geometry and function constitutes a major goal of nanoscience. Currently, the preeminent method for nanoprinting is focused electron beam-induced deposition(FEBID). During FEBID, the electron beam is scanned along a surface inducing the fragmentation and deposition of absorbed precursor molecules. Until recently, the suite of 3D objects that could be deposited was limited by the trial and-error nature of experiments and poor material quality. Our team has taken significant steps toward overcoming both roadblocks, the former being the focus of the current presentation. A FEBID CAD program will be presented that makes it possible to deposit complex, 3D nanoscale mesh style objects spanning micrometer length scales. A FEBID simulation will also be discussed. The simulation to CAD to experiment process flow will be demonstrated for the case of tailoring mesh object nanowire cross-sections.

Invited Talk KFM 16.2 Wed 10:00 H 2032

Nanosuperconductivity with Focused Particle Beam Induced Deposition structures — •Rosa Córdoba[1,2], Javier Sesé[2,3], and José María De Teresa[1,2,3] — [1]Instituto de Ciencia de Materiales de Aragón (ICMA), CSIC - Universidad de Zaragoza, Spain — [2]Departamento de Física de la Materia Condensada, Universidad de Zaragoza, 50009 Zaragoza, Spain — [3]Laboratorio de Microscopías Avanzadas (LMA), Instituto de Nanociencia de Aragón (INA), Universidad de Zaragoza, Spain

In this contribution, we will show an inclusive scenario of Focused Particle Beam Induced Deposition (FEBID/FIBID) to grow nanosuperconductors and nanomagnets by using as a primary beam, heavy ions (Ga+ FIBID), light ions (He+ FIBID) and electrons (FEBID). First, Ga+ FIBID nanosuperconductors will be introduced, which include the mechanical properties of three-dimensional (3D) nanowires [1], the non-local vortex transport in sub-50 nm nanowires [2] and the magnetotransport properties of sub-10 nm superconducting nanowires [3]. Second, He+ FIBID nanotubes will be presented, highlighting their specific growth method, superconducting properties and microstructure [4]. Finally, FEBID 3D magnets will be shown, which are integrated in a hybrid (superconductor/ferromagnet) system [5,6]. [1]Córdoba et al., Nanotechnology 28-44 445301 (2017). [2]Córdoba et al., manuscript submitted to Applied Physics Letters. [3]Córdoba et al., manuscript in preparation. [4]Córdoba et al., manuscript submitted to Nano Letters. [5]Córdoba et al., Nanotechnology 27 355301 (2016). [6]Rouco et al., Sci. Rep. 7 5663 (2017).

Invited Talk KFM 16.3 Wed 10:30 H 2032

Chemistry for ELectron-Induced NAnofabrication — •Petra Swiderek — University of Bremen, Institute for Applied and Physical Chemistry, Bremen, Germany

The European COST Action CELINA (Chemistry for ELectron- Induced NAnofabrication [1]) has, from 2013 to 2017, created a research network that aims at advancing focused electron beam induced deposition (FEBID) processes. It has done so by stimulating collaborative research that unravels the chemical reactions that are fundamental to FEBID, develops novel and improved precursor molecules, and tests their performance in the actual FEBID process. CELINA has thus assembled under its roof groups with expertise in electron-driven chemistry, precursor synthesis, and experts in FEBID from both academia and industry. This multidisciplinary effort is needed because of the many different physical and chemical aspects involved in the formation and processing of FEBID deposits as well as in their applications.

This contribution gives an overview of CELINA*s research program and highlights some of its results. Furthermore, it will discuss the different types of chemical processes inherent in FEBID and how they can be investigated using a combination of gas phase mass spectrometry and surface science experiments. Understanding and controlling each of these different chemistries poses significant challenges but is the key to ultimate deposit purity, spatial resolution, and deposition speed.

References: [1] http://celina.uni-bremen.de/celina

Invited Talk KFM 16.4 Wed 11:00 H 2032

The direct electron beam writing of plasmonic nanostructures — •Katja Höflich — Helmholtz Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, D – 14109 Berlin, Germany

Future IT systems will rely on photons instead of electrons. The potentially huge bandwidth of photons and their extremely small switching times render light indispensable for telecommunication and for information processing. The use of plasmonic nanostructures constitutes a promising approach for nanoscale optical devices since their minimum geometric features are not restricted by the diffraction limit.

The technique of electron beam induced deposition (EBID) has the potential to evolve as a novel route for the fabrication of complex plasmonic devices. EBID nanostructures are grown by the local dissociation of precursor molecules in the focus of an electron beam. While the focused electrons account for minimum structural features, the direct writing provides access to three dimensions in a single step.

A major challenge lies at depositing pure materials. It can be addressed by testing novel precursor compounds, oxidation-based purification or by using EBID nanostructures as a scaffold to be coated with the metal of choice. Recent examples of EBID-based plasmonic nanostructures include silver and gold helices with a strong dichroism in the visible range as well as silver nanostructures based on a novel carboxylate precursor.

15 min. break.

KFM 16.5 Wed 11:45 H 2032

Direct printing of 3D nano-structures via focused electron beam induced deposition: Pattern generation — •Lukas Keller and Michael Huth — Institute of Physics, Goethe University, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

Fabrication of three-dimensional (3D) nano-architectures by focused electron beam induced deposition (FEBID) has matured to a level that highly complex and functional deposits are becoming available for nanomagnetics and plasmonics. The main issue of generating a desired 3D nano-structure is the control of the electron beam in the x-y-plane. However, the generation of suitable pattern files that define the electron beam deflection at any time during the deposition and reliably map the desired target 3D structure from a purely geometrical description to a shape-conforming 3D deposit is non trivial. Here we present our implementation of a pattern file generator that handles proximity effects, corrects for height-dependent precursor coverage and avoids shadowing effects regarding the directed component of the precursor flux. Several examples of successful 3D nano-fabrication using different precursors are presented that attest the effectiveness of the implementation.

KFM 16.6 Wed 12:00 H 2032

Direct-Write Fabrication of Electric and Thermal High-Resolution Nano-Probes on Self-Sensing AFM Cantilever — •Juergen Sattelkkow[1,2], Johannes Froech[1,2], Robert Winkler[1,2], Christian Schwalb[3], Ernest Fantner[3], Vlado Stavrov[4], and Harald Plank[1,2] — [1]Institute of Electron Microscopy and Nanoanalysis, Graz University of Technology, Graz, Austria — [2]Graz Centre for Electron Microscopy, Graz, Austria — [3]GETec Microscopy Inc. & SCL Sensor.Tech. Fabrication Inc., Vienna, Austria — [4]AMGT, Botevgrad, Bulgaria

Atomic Force Microscopy (AFM) has evolved into an essential part in research and development due to its quantitative 3D surface characterization capabilities on the spatial nanoscale together with the possibility to access laterally resolved magnetic, chemical, mechanical, optical, electric or thermal properties of the sample surface. In this contribution, we demonstrate the direct-write fabrication of 3D nano-probes via focused electron beam induced deposition (FEBID) together with its respective AFM application. For conductive-AFM, Pt-C nano-pillars are initially fabricated by FEBID and then chemically transferred into pure Pt via gas assisted post-growth purification. For thermal nano-probes we use platinums temperature dependent, electric properties as transducing element together with FEBIDs 3D fabrication capabilities to realize free-standing nano-bridges. We demonstrate the reversible, quantitative temperature response together with fast response times of less than 30 ms/K. Finally, we show scanning thermal microscopy measurements, revealing thermal surface gradients on the nanoscale.

KFM 16.7 Wed 12:15 H 2032

High-Fidelity 3D-Nanoprinting via Focused Electron Beams: Growth Fundamentals — •Robert Winkler[1,2], Brett Lewis[3,4], Jason Fowlkes[3,4], Philip Rack[3,4], and Harald Plank[1,2] — [1]Institute for Electron Microscopy and Nanoanalysis Graz University of Technology, 8010 Graz, Austria — [2]Graz Centre for Electron Microscopy, 8010 Graz, Austria — [3]Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — [4]Department of Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee 37996, USA

3D-printing of functional structures has emerged to an important technology in research and development, although it becomes very challenging when aiming on nano-sized geometries. Among the very few direct-write techniques on that scale, Focused Electron Beam Induced Deposition (FEBID) has been demonstrated to be a promising candidate as it allows the fabrication of functional, freestanding 3D nano-architectures on almost any substrate, enabling novel applications. Predictable, reliable and reproducible fabrication, however, often suffered due to the numerous process parameter and their mutual relationships. In this contribution, we comprehensively discuss the complex interplay between most process parameters and successfully trace back their implications to the precursor working regime. Beside the fundamental aspect of our findings, we separate dominant parameters from those with minor implications. By that, we are able to explain unwanted deviations during 3D growth and derive certain rules for precise, predictable and reproducible 3D-nanofabrication via FEBID.

KFM 16.8 Wed 12:30 H 2032

Mechanical Properties of 3D Nano-Architectures Fabricated via Focused Electron Beam Induced Deposition — Johannes Froech[1,2], Juergen Sattelkow[1,2], Robert Winkler[1,2], Christian Schwalb[3], Ernest Fantner[3], and •Harald Plank[1,2] — [1]Institute for Electron Microscopy and Nanoanalysis Graz University of Technology, 8010 Graz, Austria — [2]Graz Centre for Electron Microscopy, 8010 Graz, Austria — [3]GETec Microscopy Inc. & SCL Sensor.Tech. Fabrication Inc., 1220 Vienna, Austria

With the recent introduction of controlled 3D nano-printing via focused electron beam induced deposition, an entirely new range of applications such as nano-optics, -mechanics, or -electronics comes within reach whose fabrication is extremely challenging or even impossible with alternative techniques. In this contribution, we focus on mechanical properties of freestanding, Pt based 3D nano-architectures for atomic force microscopy (AFM) based application as high-resolution thermal nano-probes. A combined approach of finite element simulation, AFM based force spectroscopy and real-time imaging via scanning electron microscopy is used to identify and compensate highly unwanted peculiarities. In more detail, we discuss an unexpectedly strong influence of non-straight side branches as well as the consequences of fabrication mismatches on the lowest nanoscale, leading to non-linear mechanical behaviour and morphological twisting, respectively. The combined outcome of our findings demonstrate the high demands on nanoscale accuracy during 3D nano-printing to exploit the full potential in terms of predictable mechanical properties.

KFM 16.9 Wed 12:45 H 2032

Correlative in-situ characterization of 3D nanostructures by combining SEM and AFM — •Christian Schwalb[1], Marcel Winhold[1], Pinar Frank[1], Stefan Hummel[1], Roland Sachser[2], Michael Huth[2], Jürgen Sattelkow[3], and Harald Plank[3] — [1]GETec Microscopy GmbH, Vienna, Austria — [2]Physikalisches Institut, Goethe University Frankfurt, Germany — [3]FELMI, Graz, Austria

Focused electron-beam-induced processing represents one of the most flexible approaches for functional nanostructure fabrication. During and after the growth process, e.g., electrical in-situ measurements as well as energy-dispersive X-ray spectroscopy are commonly employed to characterize electrical and chemical properties of fabricated structures. However, one major drawback is the lack of further in-situ analysis tools which grants access to real 3D topographic information, laterally resolved conductance maps, local magnetic or mechanical properties. We present a novel AFM that allows correlative in-situ analysis by combining the full SEM and AFM capability. The AFM measurement takes place in the field of view of the electron beam and thus allows for non-destructive and non-contaminating analyses of FEBID structures directly after fabrication. We make use of novel self-sensing cantilevers that are equipped with different specialized tips fabricated by 3D nano-printing of sharp purified metallic or magnetic tips. We present correlative in-situ conductive, magnetic and mechanical analysis of 3D nanostructures using these novel cantilever tips and discuss future applications.

KFM 17: Skyrmions III (joint session MA/TT/KFM)

Time: Wednesday 15:00–18:30 Location: EB 301

KFM 17.1 Wed 15:00 EB 301

Skyrmion drag effect: — •Adel Abbout[1], Joseph Weston[2], Xavier Waintal[2], and Aurelien Manchon[1] — [1]King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia — [2]CEA Grenoble, France.

In this work, we study the motion of skyrmionic magnetic textures and analyze the current induced by this motion using time-dependent non-equilibrium Green's function formalism implemented on a real-space tight-binding model. We focus on the time dependent distribution of the nonequilibrium charge and spin densities and discuss the corresponding topological Hall effect. The perturbation induced by this motion applies a torque on the whole texture. The influence of the generated current on the whole texture is discussed and its signature is unveiled in the renormalization of the damping parameter. A cooperative effect due to the collective motion of skyrmions is proposed in order to enhance the skyrmion's velocity. The stationary regime is analyzed as a function of the different parameters of the system and explained using the formalism of electronic pumping. A simple formula for the current is proposed.

KFM 17.2 Wed 15:15 EB 301

Theory of tunneling vector spin transport on a magnetic skyrmion — •Krisztián Palotás[1,2], Levente Rózsa[3], and László Szunyogh[4] — [1]Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia — [2]University of Szeged, Szeged, Hungary — [3]University of Hamburg, Hamburg, Germany — [4]Budapest University of Technology and Economics, Budapest, Hungary

Spin-polarized scanning tunneling microscopy (SP-STM) demonstrated the creation and annihilation of individual magnetic skyrmions [1] that is promising for future technological use. The detailed microscopic mechanisms for these processes are, however, unknown. In the present work the tunneling spin transport of a magnetic skyrmion is theoretically investigated in SP-STM. The spin-polarized charge current [2] and tunneling spin transport vector quantities, the longitudinal spin current and the spin transfer torque are calculated in high spatial resolution within a simple electron tunneling theory for the first time. Beside the vector spin transport characteristics, the connections between conventional charge current SP-STM images and the magnitudes of the spin transport quantities are analyzed.

[1] N. Romming et al., Science 341, 636 (2013).
[2] K. Palotás et al., Phys. Rev. B 96, 024410 (2017).

KFM 17.3 Wed 15:30 EB 301

Quantum dynamics of skyrmions in chiral magnets — •Christina Psaroudaki — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

We study the quantum propagation of a skyrmion in chiral magnetic insulators by generalizing the micromagnetic equations of motion to a finite temperature path integral formalism, using field theoretic tools. Promoting the center of the skyrmion to a dynamic quantity, the fluctuations around the skyrmionic configuration give rise to a time-dependent damping of the skyrmion motion. From the frequency dependence of the damping kernel, we are able to identify the skyrmion mass, thus providing a microscopic description of the kinematic properties of skyrmions. When defects are present or a magnetic trap is applied, the skyrmion mass acquires a finite value proportional to the effective spin, even at vanishingly small temperature. We demonstrate that a skyrmion in a confined geometry provided by a magnetic trap behaves as a massive particle owing to its quasi-one dimensional confinement. An additional quantum mass term is predicted, independent of the effective spin, with an explicit temperature dependence which remains finite even at zero temperature.

KFM 17.4 Wed 15:45 EB 301

Optimizing the size of long-lived magnetic skyrmions — Anastasiya Varentsova[1], Stephan v. Malottki[2], Stefan Heinze[2], and •Pavel F. Bessarab[1,3] — [1]ITMO University, St. Petersburg, Russia — [2]University of Kiel, Kiel, Germany — [3]University of Iceland, Reykjavik, Iceland

Available experimental data on magnetic skyrmions in various materials demonstrate inverse correlation between the skyrmion size and skyrmion stability: small skyrmions tend to be less stable compared to large ones [1,2]. The question arises how fundamental this trend is and whether it is possible to obtain long-lived magnetic skyrmions at ambient conditions while keeping their size at the nanoscale.

Here, we demonstrate by means of transition state theory [3] and minimum energy path calculations [4] that the skyrmion lifetime at a given temperature is not a unique function of the skyrmion size and that it is possible to systematically tune material parameters so as to minimize the size of skyrmions while keeping their stability at a desired level. Based on this analysis we identify the most promising materials for the use as storage media based on magnetic skyrmions.

[1] W. Jiang *et al.*, Science **349**, 283 (2015).
[2] N. Romming *et al.*, Science **341**, 636 (2013).
[3] P.F. Bessarab *et al.*, Phys. Rev. B **85**, 184409 (2012).
[4] P.F. Bessarab *et al.*, Comput. Phys. Commun. **196**, 335 (2015).

KFM 17.5 Wed 16:00 EB 301

Critical Phenomena in Confined Skyrmion Systems — •Jonathon Waters[1], Timothy Sluckin[1], Denis Kramer[1], Hans Fangohr[2], and Ondrej Hovorka[1] — [1]University of Southampton, Southampton, UK — [2]European XFEL, Germany

There have been extensive studies which establish the magnetic phases and quantify the thermal phase transition behaviour in bulk helimagnetic materials. However, many proposed device applications, which will utilise the skyrmion phase of these materials, are expected to assume operation in confined geometries and, therefore, it is critical to access the role of the confinement and finite size effects on the stability of skyrmion phases. So far, there have been few studies aimed at understanding the finite system size effects on the thermal phase transition behaviour in these systems. This presentation will discuss our recent developments of systematic analysis of these fundamental effects.

We present large-scale Monte-Carlo simulations of cubic nanoparticles, modelled by a general Heisenberg model with Dzyaloshinskii-Moriya interaction (DMI), and establish phase diagrams for different combinations of exchange and DMI strengths. We apply several different annealing protocols when generating the phase diagram in order to establish the role of metastability and hysteresis in the phase behaviour of these systems. Finally we discuss the results of a finite system size scaling analysis and establish the dependence of critical phase transition temperature on the particle size.

KFM 17.6 Wed 16:15 EB 301

Magnetic skyrmion dynamics in thin cylindrical nanodots — •Konstantin Guslienko[1,2] and Zukhra Gareeva[3] — [1]Depto. Física de Materiales, Universidad del País Vasco, UPV/EHU, 20018 San Sebastián, Spain — [2]IKERBASQUE, the Basque Foundation for Science, 48013 Bilbao, Spain — [3]Institute of Molecule and Crystal Physics, Russian Academy of Sciences, 450075 Ufa, Russia

Magnetic skyrmions, robust particle-like nanosize objects, attracted considerable attention due to promising applications in spintronics and information technologies. Being a kind of magnetic topological solitons in 2D spin systems, skyrmions exhibit a wide variety of unusual properties related to their topology. In this talk we focus on the low and high frequency dynamics of magnetic skyrmions in the systems of restricted geometry: isolated cylindrical nanodots. We consider Bloch- and Neel skyrmions as the ground magnetic state of thin circular nanodots stabilized due to an interplay of the isotropic and Dzyaloshinskii-Moriya exchange interactions, perpendicular magnetic anisotropy and magnetostatic interaction. We calculate spectrum of spin excitations over the skyrmion background and classify the eigenmodes according to their spatial symmetry. We show that only one gyrotropic mode (rotation of the skyrmion center position with the frequency about of 1 GHz) exists for the skyrmion of definite polarity and the other low frequency modes that are observed in the skyrmion excitation spectra correspond to spin waves. We found an asymmetry between azimuthal spin waves propagating in the clockwise and counter-clockwise directions that is closely related to the skyrmion topology.

KFM 17.7 Wed 16:30 EB 301

Internal structure and stability of skyrmions in ferromagnet/heavy-metal multilayers — •Ksenia Chichay[1], Joseph Barker[2], and Oleg Tretiakov[2,3] — [1]Center for Functionalized Magnetic Materials (FunMagMa), Immanuel Kant Baltic

Federal University, Kaliningrad, Russia — [2]Institute for Materials Research, Tohoku University, Sendai, Japan — [3]School of Natural Sciences, Far Eastern Federal University, Vladivostok, Russia

Magnetic Skyrmions are one of the fascinating and promising objects because of their small size and stability to perturbations such as electric currents and magnetic fields. The major mechanism to stabilize small skyrmions in ferromagnet/heavy-metal bilayers is the presence of Dzyaloshinskii-Moriya interaction (DMI).

In this work we investigate the stability and internal structure of an isolated skyrmion in bilayer (ferromagnet/heavy metal) and trilayer (heavy metal 1/ferromagnet/heavy metal 2) nanodisks. We study the static properties of the skyrmions and obtain the phase diagrams of the skyrmion existence depending on the thickness of the ferromagnetic layer and the DMI strength. We demonstrate the importance of fully taking into account the dipolar interaction even for a few atomic layers thin nanodisk and that together with DMI it has the stabilizing effect and defines the Skyrmion configuration. For the trilayer structures with two heavy-metal interfaces, we show that the type and configuration of the skyrmion can be controlled by the thickness of ferromagnet. Furthermore, the interplay of two interfacial DMIs can lead to the formation of magnetic structures with higher winding number.

KFM 17.8 Wed 16:45 EB 301

Skyrmion dynamics under the influence of defects from DFT to ASD — •Jonathan Chico, Imara Lima Fernandes, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

Any potential skyrmionic application must be able to handle the impact of defects on the movement of skyrmions. Until now, most approaches focussed on large skyrmions and thus phenomenological schemes in the micromagnetic regime. In this work we discuss the technologically much more promising small skyrmions.

Using a combination of first-principles calculations and atomistic spin dynamics, the motion of small skyrmions in Pd/Fe/Ir(111) with 3*d* and 4*d* atomic defects is studied. In general, two types of defects are found, attractive and repulsive [1]. It can be observed that depending on the chemical nature of the defect the current threshold needed to overcome the energy barriers, resulting from the impurities, varies. The obtained dynamical behaviour is richer than what is expected from the Thiele equation. The complexity of the different motion regimes are revealed and compared with what is known for larger skyrmions. The present study also shines light on how one can engineer defects-based pathways for controlled skyrmion motion.

[1] I. L. Fernandes *et al.* submitted (2017).

Funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC-consolidator grant 681405 - DYNASORE).

KFM 17.9 Wed 17:00 EB 301

First-principles study of skyrmion formation at 3*d*/4*d* transition-metal interfaces — •Soumyajyoti Haldar[1], Stephan von Malottki[1], Pavel F. Bessarab[2], and Stefan Heinze[1] — [1]Institute of Theoretical Physics and Astrophysics, University of Kiel, 24098, Kiel, Germany — [2]School of Engineering and Natural Sciences, University of Iceland, 107, Reykjavik, Iceland

Typically, it is assumed that for the formation of skyrmions with a diameter of a few nanometers a 3*d*/5*d* transition metal (TM) interface is required due to the large spin-orbit coupling of heavy TMs which leads to large Dzyaloshinskii-Moriya interaction (DMI). Here, we use density functional theory (DFT) as implemented in the FLEUR code [1] to demonstrate that ultrasmall skyrmions can also emerge at 3*d*/4*d* TM interfaces. We have calculated the magnetic interactions in atomic bilayers of Pd/Fe on the Rh(111) surface – a system which is similar to Pd/Fe/Ir(111) [2, 3] since Rh and Ir are isoelectronic 4*d*- and 5*d*-TMs. From our DFT calculations we parametrize an atomistic spin model including exchange interactions, DMI and the magnetocrystalline anisotropy energy (MAE). We find that both DMI and MAE are reduced with respect to Pd/Fe/Ir(111) which still allows a spin spiral phase at zero magnetic field due to DMI. Using spin dynamics simulations we find that a skyrmion phase occurs for both fcc and hcp stacking of the Pd layer at small magnetic fields of ~ 1 T. Depending on the stacking the skyrmion diameters amount to 4 to 6 nm.

[1] http://www.flapw.de [2] N. Romming *et al.*, Science **341**, 6146 (2013) [3] B. Dupé *et al.*, Nature Comm. **5**, 4030 (2014).

KFM 17.10 Wed 17:15 EB 301

Frustration of the Dzyaloshinskii-Moriya interaction in ultrathin Co films — •Sebastian Meyer[1], Stephan Von Malottki[1], Bertrand Dupé[2], and Stefan Heinze[1] — [1]Institute of Theoretical Physics and Astrophysics, Christian-Albrechts-Universität zu Kiel, Leibnizstrasse 15, 24098 Kiel — [2]Institute of Physics, Johannes Gutenberg Universität Mainz, Staudingerweg 7, 55128 Mainz

Non-collinear spin structures such as chiral domain walls and skyrmions are being intensively studied since they are promising for spintronic applications [1, 2]. The Dzyaloshinskii-Moriya interaction (DMI) is crucial for stabilizing these non-trivial magnetic states favoring a unique rotational sense. Here, we show frustration of the DMI in ultrathin Co films using density functional theory (DFT) as implemented in the FLEUR code [3]. We study Co monolayers and Pt/Co bilayers on the Ir(111) surface and calculate the energy dispersion of homogeneous flat spin spirals including spin-orbit coupling. Clockwise rotating spin spirals are preferred for large periods close to the ferromagnetic state while below a certain spin spiral period an anticlockwise sense is obtained. This effect arises due to competing DMI interactions with different neighbors that are of opposite sign. With our results from DFT, we parametrize an atomistic spin model and simulate domain wall properties using spin-dynamics simulations.

[1] S. S. P. Parkin *et al.*, Science **320**, 190 (2008)
[2] A. Fert *et al.*, Nature Nano. **8**, 152 (2013)
[3] www.flapw.de

KFM 17.11 Wed 17:30 EB 301

Isolated skyrmions with vanishing anisotropy in Co/Ru(0001) — •Marie Böttcher[1,2], Marie Hervé[3], Jairo Sinova[1,4], Wulf Wulfhekel[3], and Bertrand Dupé[1] — [1]Johannes Gutenberg-Universität Mainz, Mainz, Germany — [2]Graduate School Materials Science in Mainz, Mainz, Germany — [3]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [4]Academy of Sciences of the Czech Republic, Praha, Czech Republic

Magnetic skyrmions are localized and topologically stabilized non-collinear spin structures. They offer attractive perspectives for future spintronics applications, because they can be manipulated at lower current densities than domain walls [1]. The stabilization of skyrmions is usually attributed to a large Dzyaloshinskii-Moriya interaction (DMI). Here, we show that a strong DMI is not a necessary condition to obtain skyrmions in ultra-thin films. Co/Ru(0001) possesses a spin spiral ground state, although the DMI is weak. We attribute the stability of this spin texture to the simultaneous vanishing of anisotropy [2]. We determine the B-T phase diagram for this system using Monte Carlo simulations and show the magnetic field dependence of isolated skyrmions at magnetic fields with a ferromagnetic ground state. [1] A. Fert, *et al.* Nature Nano. **8**, 152 (2013). [2] M. Hervé *et al.* arXiv:1707.08519 (2017)

KFM 17.12 Wed 17:45 EB 301

Magnetic skyrmions in curvilinear films — •Volodymyr Kravchuk[1,2], Denis Sheka[3], Attila Kakay[4], Oleksii Volkov[4], Ulrich Roessler[1], Jeroen van den Brink[1], Denys Makarov[4], and Yuri Gaididei[2] — [1]Leibniz-Institut fuer Festkoerper- und Werkstoffforschung, D-01171 Dresden, Germany — [2]Bogolyubov Institute for Theoretical Physics of National Academy of Sciences of Ukraine, 03680 Kyiv, Ukraine — [3]Taras Shevchenko National University of Kyiv, 01601 Kyiv, Ukraine — [4]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Topological magnetic solitons on curvilinear magnetic films acquire new properties if the curvature radius is comparable with the size of the soliton. Earlier we demonstrated [1] that ferromagnetic skyrmions can be stabilized due to the curvature effects only without intrinsic chiral magnetic interactions. However, the curvature induced skyrmion is an excitation of the ground state, as well as a skyrmion in a planar film. Here we show that the combined action of the curvature and the chiral interaction can make skyrmion the ground state of the system [2]. Moreover, ferromagnetic skyrmion pinned on a curvilinear defect demonstrates a discrete set of equilibrium states. Transitions between different states can be controlled by external magnetic field. Thus, the periodically arranged curvilinear defects can result in a reconfigurable skyrmion lattice. This opens new perspectives on processing and storing of the information.

[1] V. Kravchuk et al., BRB 94, 144402 (2016). [2] V. Kravchuk et al., arXiv 1706.05653 (2017).

KFM 17.13 Wed 18:00 EB 301

Skyrmion-Lattice Collapse and Defect-Induced Melting in Chiral Magnetic Films — •Leonardo Pierobon[1], Christoforos Moutafis[2], Michalis Charilaou[1], and Jörg Löffler[1] — [1]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Switzerland — [2]School of Computer Science, University of Manchester, Manchester, UK

Complex spin textures arise in nanostructured magnets due to competing interactions, primarily the Heisenberg exchange and the Dzyaloshinskii-Moriya interaction (DMI), which promote spin collinearity and canting, respectively. Upon rotational-symmetry breaking, particle-like objects with non-trivial spin configurations, i.e., skyrmions, can be created. The winding of skyrmions bestows a topological protection on the system, and the transition to the topologically trivial ferromagnetic state requires a phase transition. Here, we systematically compare isotropic and anisotropic DMI systems by means of high-resolution numerical simulations. We show that in perfect systems skyrmion lattices can be inverted in a field-induced first-order phase transition, whereas the existence of even a single defect replaces the inversion with a second-order phase transition following a defect-induced lattice melting process. This radical qualitative change signifies the importance of employing such an analysis for all realistic systems in order to correctly interpret experimental data. Our results shed light on fundamental processes behind magnetic phase transitions, and pave the way for their experimental realization in technologically relevant multilayer materials.

KFM 17.14 Wed 18:15 EB 301

Reservoir Computing with Random Skyrmion Fabrics — •Daniele Pinna[1], George Bourianoff[2], and Karin Everschor-Sitte[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Mainz, Germany — [2]Intel Labs, Intel Corp, Austin, TX

Thanks to their many nanoscale properties, skyrmions are promising in applications ranging from non-volatile memory[1] and spintronic logic devices[2], to enabling the implementation of unconventional computational standards[3, 4]. In this talk we will discuss how a random skyrmion "fabric" composed of skyrmion clusters embedded in a magnetic substrate can be effectively employed to implement a functional reservoir computer. This is achieved by leveraging the nonlinear resistive response of the individual skyrmions arising from their current dependent AMR[5]. Complex time-varying current signals injected via contacts into the magnetic substrate are shown to be modulated nonlinearly by the fabric's AMR due to the current distribution following paths of least resistance as it traverses the geometry. By tracking resistances across multiple input and output contacts, we show how the instantaneous current distribution, reminiscent of Atomic Switch Networks, effectively carries temporally correlated information about the injected signal. This in turn allows us to numerically demonstrate simple pattern recognition.

[1] A. Fert, et al., Nature Nanotech. 8, 152-156 (2013). [2] X. Zhang, et al., Sci. Rep. 5, 9400 (2015). [3] D. Pinna, et al., arXiv:1701.07750 (2017). [4] G. Bourianoff, et al., arXiv:1709.08911 (2017). [5] D. Prychynenko, et al., arXiv:1702.04298 (2017).

KFM 18: Diamond II + Poster

This dedicated focus session represents the production and applications of diamond and diamond related materials in the fields of dielectrics, electronics, high frequency techniques, GHz-THz- applications, mechanics and optics. Also materials/composites like carbides, boron-carbides and nitrides are related materials with excellent mechanical properties. Applications with integrated diamond or related materials in technical systems are part of this session (Nuclear fusion applications,high frequency heating systems and material processing).

Chair: Theo Scherer KIT Karlsruhe

Time: Wednesday 15:00–17:30 Location: E 124

Invited Talk KFM 18.1 Wed 15:00 E 124

Application of Diamond Technology to Microwave Systems in Nuclear Fusions Machines — •Giovanni Grossetti, Gaetano Aiello, Francesco Mazzocchi, Andreas Meier, Sabine Schreck, Peter Spaeh, Dirk Strauss, and Theo Scherer — Karlsruhe Institute of Technology (Institute of Applied Materials), P.O. Box 3640 76021 Karlsruhe Germany

The growing energy demand, set to increase by 37% by 2040, and the reduction of greenhouse gases are two key reasons why the energy landscape needs to be less reliant on fast-depleting fossil fuels. In this frame, Nuclear Fusion represents an option by being a nearly unlimited, safe and CO2-free friendly energy source. In order to reach and support the required conditions such that nuclear fusion reaction can occur, a gas mixture (deuterium and tritium) needs to be confined, e.g. through strong magnetic fields, and heated using microwave systems operating at the cyclotron frequency. Such systems shall meet several requirements from both the physics and the engineering point of view and make use of diamond disks grown by Chemical Vapor Deposition (CVD). In this paper we present an overview of the applications of such disks in components know as diamond windows, for both present machine and ITER, and future power plants.

KFM 18.2 Wed 15:30 E 124

Application of CVD Diamond Discs in High Power Fusion Gyrotrons and Power Plants — •Sebastian Ruess[1,2], Gaetano Aiello[3], Gerd Gantenbein[1], Manuel Gärtner[1], Tomasz Rzesnicki[1], Theo Scherer[3], Dirk Strauss[3], Manfred Thumm[1,2], Jörg Weggen[1], and John Jelonnek[1,2] — [1]IHM, — [2]IHE, — [3]IAM-AWP, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

Karlsruhe Institute of Technology (KIT) is doing research and development in the field of megawatt-class RF sources (gyrotrons) for the Electron Cyclotron Resonance Heating (ECRH) systems of the International Thermonuclear Experimental Reactor (ITER) and the DEMOnstration Fusion Power Plant that will follow ITER. In the focus is the development and verification of the European coaxial-cavity gyrotron technology which shall lead to gyrotrons operating at an RF output power significantly larger than 1 MW CW and at an operating frequency up to 240 GHz.

Currently, the KIT is working on high-power broadband microwave output window systems for strongly overmoded waveguides based on ultra-low loss CVD-diamond. The ongoing research is focusing on the electromagnetic properties in combination with the manufacturing of very large windows (up to 180 mm) and the development of advanced technologies for joining of large diamond discs for advanced broadband CVD Brewster-angle windows. The simulation of the electrical large structures is requiring specific care. This presentation will focus on the related multiphysics simulations using the commercial tool CST.

KFM 18.3 Wed 15:50 E 124

Diamond Window Diagnostics For Fusion Applications — •Francesco Mazzocchi, Gaetano Aiello, Dirk Strauss, Andreas Meier, and Theo Scherer — KIT IAM AWP Hermann von Helmholtz Platz 1 76344 Eggenstein Leopoldshafen

The future nuclear fusion power plants will require Electron Cyclotron Heating and Current Drive (ECH&CD) systems to heat up and stabilize the plasma inside the vacuum vessel. One of the key components of such systems is the Chemical Vapor Deposition (CVD) diamond window. In this work, the latest assessment study on a set of diagnostics to be part of the window assembly is shown. The required diagnostics include arc and tritium detection, microwave stray radiation (perpendicular to the main beam and generated by cracks in the windows), pressure and disk temperature measurements. The devices must have a compact, simple and flexible layout, with a rugged design, to maximize serviceability and durability. To accommodate the diagnostics previously mentioned, a new design for the window housing was devel-

oped. To validate the concepts, a test bench was developed to carry out measurements under conditions similar to the operative ones.

KFM 18.4 Wed 16:10 E 124

Loss mechanisms of microwave and THz radiation in poly and single crystalline diamond — •Theo Scherer — Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

To understand the microwave and THz wave propagation in poly and single crystalline diamond, the losses caused by free charge carrier absorption, dipole relaxation, phonon resonance absorption and disorder absorption will be discussed. The main loss parameter in such dielectrics is the loss tangent. Intergrain scattering effects in polycrystalline diamond are a limiting factor for further reduction of losses in that materials. The way to come to losses of < 10E-6 in loss tangent will be shown and discussed. One important application of low loss diamond in disk shape is the transmission of Megawatt power for plasma heating in future fusion reactors as electrical power plants.

KFM 18.5 Wed 16:30 E 124

Influence of WC-Co on the High-Frequency Properties of Soft Ferromagnetic Fe-Co-Hf-N Films Used for Sensor Application — •Stefan Beirle, Klaus Seemann, and Harald Leiste — Karlsruhe Institute of Technology (IAM-AWP), 76344 Eggenstein-Leopoldshafen, Germany

The thermal and mechanical induced high frequency property changes of soft ferromagnetic Fe-Co-Hf-N films with an in-plane uniaxial anisotropy are promising for the application for sensor systems. For example, one can use the sensor signal to measure the cutting tool temperature during metal processing. Consequently, it is necessary to investigate how the ferromagnetic film interacts with a cemented carbide substrate, which is typically used for cutting tools, but consists itself of a hard ferromagnetic Co phase. In order to overcome the exchange interactions between the substrate and the ferromagnetic film, it is possible to predeposit a non-ferromagnetic buffer layer on the WC-Co substrate. For this purpose different hard coatings like Ti-N, Ti-Al-N and an electrically insulating Si-O buffer layer were investigated. In order to determine the static and dynamic magnetic properties of the film, MOKE measurements were carried out as well as the complex permeability was determined. The buffer materials show a different decoupling behaviour regarding the high frequency permeability due to different electrical and microstructural properties. The decoupled films show ferromagnetic resonance absorbance and the FWHM of the resonance line can be tuned by increasing the electrically insulating buffer layer thickness.

KFM 18.6 Wed 16:50 E 124

Mechanical load study on Diamond Window Mock-up — •Andreas Meier, Theo Scherer, Gaetano Aiello, Giovanni Grossetti, Francesco Mazzocchi, Sabine Schreck, and Dirk Strauss — KIT Karlsruhe, 76344 Eggenstein-Leopoldshafen, Germany

An Electron Cyclotron Heating (ECH) is an effective heating system in nuclear fusion reactors. The power transfer of the microwave radiation into the torus is realized by diamond windows which are relevant components for the retention of tritium. Mechanical stability and leak tightness are essential characteristics. A mock-up, consisting of a large diamond disk, diameter 80mm and thickness 1.11mm, brazed on cylindrical copper cuffs (diameter 70mm) was tested under different pressure scenarios and cyclic loads. Leak tightness measurements identified leak rates directly by using helium gas.

KFM 18.7 Wed 16:50 E 124

Torus Diamond Window for ITER - R&D and Qualification activities for a Protection Important Component — •Sabine Schreck, Gaetano Aiello, Stefan Dieterle, Andreas Meier, Dirk Strauss, and Theo Scherer — Karlsruher Institut für Technologie

The diamond window is part of the ITER ECRH Upper Launcher system and consists of an ultra-low loss CVD diamond disk mounted in a system of metallic parts. The window has to fulfil adequate transmission capability for high power mm-waves and it serves as primary vacuum and tritium boundary of the ITER vacuum vessel. Classified as Protection Important Component high requirements for quality and safety apply. As the window cannot be entirely covered by codes and standards an ad-hoc qualification program is required, including prototyping and previous R&D. Diamond disks with a low dielectric loss tangent <2*10-5), a diameter of 65 mm and a thickness of 1.11 mm are planned to be integrated into the window housing. This thickness satisfies the resonance condition for the 170 GHz beam, ensuring a high transmission. But the disks also need to be validated with respect to the mechanical loads, especially to the pressure loads. R&D activities have been performed with the aim to verify the resistance of the disk against these loads. Flexural strength measurements of diamond disks (D = 30 mm, d = 1.11 mm) have been executed using a ring to ring set-up, giving information on the failure behaviour. Further, high pressure tests up to 2 bar of a mock-up (disk brazed to a copper cuff) are under examination.

KFM 18.8 Wed 16:50 E 124

Hybrid-UV-Vis-Detektoren aus Silizium-Fotodioden und darüberliegenden polykristallinen Diamantschichten — •Alexander Lawerenz[1], Mario Bähr[1], Ralf Röder[1], Nicolas Wöhrl[2] und Volker Buck[2] — [1]CiS Forschungsinstitut für Mikrosensorik GmbH, Konrad-Zuse-Str. 14, D-99099 Erfurt — [2]Universität Duisburg-Essen, Fakultät für Physik, Lotharstr. 1, 47057 Duisburg

Es wurde ein Detektor entwickelt und hergestellt, der gleichzeitig und unabhängig UV-Licht mit Wellenlängen < ca. 230 nm und sichtbares Licht (bis in den UV-C-Bereich) detektiert. Dazu wurden auf 100 mm großen Siliziumwafern Siliziumfotodioden und darüberliegend UV-Photoresistoren, bestehend aus strukturierten 20 um dicken polykristallinen Diamantschichten, monolithisch aufgebaut. Es wurde ein Prozessschritt entwickelt, der einerseits das Substrat mit der aktiven Diodenstruktur vor der Diamantprozessierung schützt und die beiden Sensoren isoliert, andererseits aber das einfache Freilegen der Kontakte für die Siliziumdiode nach der Diamantprozessierung ermöglicht. Es gelang mittels einer 100 nm dicken Aluminiummaske, die 20 um dicken Diamantschichten mittels Sauerstoff-Plasmaätzen zu strukturieren, ohne dass das frei geätzte Substrat sichtbar geschädigt wurde. Des Weiteren konnte als Metallisierung das Ti/Au-Kathodenzerstäuben etabliert werden, die auf den relativ rauen Diamantoberflächen eine ausreichend gute Haftung mit einem geringen Kontaktwiderstand ermöglicht.

KFM 18.9 Wed 16:50 E 124

Diamant und ägyptische Pyramiden — •Peter-Michael Wilde — DE-15711 Königs Wusterhausen

Zwischen den Dimensionen der Diamantstruktur [1] und der äußeren Gestalt ägyptischer Pyramiden [2] liegen 11 Größenordnungen.

Es wird gezeigt, dass trotz dieser großen Unterschiede zwischen beiden Objektgruppen ein enger Zusammenhang besteht. Die Zahl Quadratwurzel aus 2 spielt hierbei die maßgebliche Rolle.

Zu Beginn dieses Jahrhunderts ist es in Berlin gelungen, Kristalle mit dem Habitus ägyptischer Pyramiden im System Kohlenstoff-Silicium-Germanium auf einem Siliciumsubstrat im Mikrometer-Maßstab nachzubilden.

[1] W. Kleber, H.-J. Bautsch, J. Bohm, Einführung in die Kristallographie, Verlag Technik Berlin München (1990) [2] F. Müller-Römer, Der Bau der Pyramiden im Alten Ägypten, Utz Verlag (2011)

KFM 18.10 Wed 16:50 E 124

Cross-sectional Microstructure, Stress Gradients, and Mechanical Properties in Diamond Films Revealed by X-ray Nanodiffraction and Microcantilever Testing — David Gruber[1], •Nicolas Wöhrl[2], Hadwig Sternschulte[3], Manfred Burghammer[4], Juraj Todt[5], and Jozef Keckes[1] — [1]Department für Materialphysik, Montanuniversität Leoben, Austria — [2]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [3]Fakultät für Allgemeinwissenschaften, Hochschule Augsburg, Germany — [4]ESRF, Grenoble, France — [5]Erich-Schmidt-Institut, Austrian Academy of Sciences, Leoben, Austria

Ultrananocrystalline diamond (UNCD) films consist of randomly oriented diamond grains embedded in an amorphous C:H matrix. Usually, the grain size is determined by XRD or TEM, revealing information from the total UNCD film or only locally from selected areas with low statistics. Here, we present a cross-sectional X-ray nanodiffraction study of diamond multi-layers with varying grain size from microcrystalline diamond to UNCD. X-ray nanodiffraction was performed in transmission geometry using a beam diameter of 30 nm. The sample was scanned in equidistant steps, revealing depth gradients of texture, grain size and residual stress. Young's modulus and fracture stress in both UNCD and microcrystalline sublayers were measured with micro cantilevers fabricated by FIB milling. A cross-sectional nanoindenter-based mapping of Young's modulus was carried out on a slice of the layer system prepared by FIB. The results show complex gradients of microstructure, stress state and mechanical properties.

KFM 19: Materials for Energy Storage II (joint session KFM/CPP)

Organizer: Martin Diestelhorst - Martin-Luther-Universität Halle-Wittenberg - Halle

Time: Wednesday 15:00–17:50 Location: EMH 025

Invited Talk KFM 19.1 Wed 15:00 EMH 025

Electrical double layer capacitors, Insights from fundamental research and their impact on storage devices — •Gudrun Reichenauer — Bavarian Center for Applied Energy Research, 97074 Wuerzburg, Germany

Electrical double layer capacitors (EDLC) are important components in the toolbox of currently available electrical storage devices, serving in particular applications that require reliability and high power density, such as e.g. emergency doors in airplanes, or high cycling stability at low to medium energy density, such as electrically driven buses for public transportation. Typically, optimization of EDLCs is performed by empirical tests of different active materials, binders and conductive additives. However, only limited systematic studies are available to address questions, such as

What are the optimized structures in terms of pore sizes and porosity of the active component?

How do the micropore (pores < 2 nm) characteristics affect the storage in the presence of organic, aqueous and polymer electrolytes?

What is the impact of the device layout vs. the properties of the electrode itself on the performance (energy and power density) of an EDLC?

The talk will address some of these questions using model carbon materials that allow systematic variation of key parameters and also show how new in-situ/in-operando techniques can further support a more targeted development of EDLC storage devices for different types of applications.

KFM 19.2 Wed 15:30 EMH 025

Pyrolytic graphite electrodes intercalated by $AlCl_4$ anions probed by X-ray tomography and small angle X-ray scattering — •Giorgia Greco[1], Giuseppe Elia[2], Dragomir Tachev[3], Armin Hoell[1], Robert Hahn[4], and Simone Raoux[1,5] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Str. 15, 12489 Berlin, Germany — [2]. Technische Universität Berlin, Research Center of Microperipheric Technologies, Gustav-Meyer-Allee 25, 13355 Berlin, Germany — [3]Institute of Physical Chemistry, Bulgaria Academy of Science, Acsd. G. Bonchev Str. Bl.11, 1113 Sofia, Bulgaria — [4]. Fraunhofer-Institut für Zuverlässigkeit und Mikrointegration , Gustav-Meyer-Allee 25, 13355 Berlin, Germany — [5]. Department of Physics, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

Due to the cost and limited resources of lithium, the use of Li-ion batteries for large scale applications is nowadays under discussion. Aluminum based secondary batteries could be a viable alternative to the present Li-ion technology because of their high volumetric capacity. Additionally, the low cost aluminum makes these devices appealing for large-scale electrical energy storage. We report the structural characterization by a combination of x-ray tomography and SAXS (Small Angle X-ray Scattering) related to electrochemical performances of aluminum tetrachloride electrolyte in an aluminum/graphite battery. The aim of this work is to characterize the micro- and nano-structure of highly ordered graphite during the electrochemically induced reaction mechanism of $AlCl_4$ intercalation.

KFM 19.3 Wed 15:50 EMH 025

Structural and microstructural evolution during oxygen intercalation in $Pr_2NiO_{4.25}$ single crystal investigated by in-situ synchrotron diffraction — •Avishek Maity[1,2], Rajesh Dutta[3], Monica Ceretti[3], Dmitry Chernyshov[4], and Werner Paulus[3] — [1]Institut für Physikalische Chemie, Georg-August Universität Göttingen, 37077 Göttingen, Germany — [2]Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), 85748 Garching, Germany — [3]Institut Charles Gerhardt, Université de Montpellier, 34095 Montpellier, France — [4]The European Synchrotron-ESRF, 38000 Grenoble, France

Pr_2NiO_{4+x} is a promising oxygen membrane material having excellent ionic conductivity at moderate T. Oxygen diffusion occurs through interstitial sites via phonon assisted diffusion mechanism. We found $Pr_2NiO_{4.25}$ to be structurally extremely complex, showing large oxygen (interstitial) and charge (Ni^{2+}/Ni^{3+}) ordered domains, and forming giant unit cells up to 6000000 $Å^3$. In order to explore the oxygen diffusion from structural and microstructural aspect as a function of oxygen stoichiometry ($0<x<0.25$), we investigated in-situ electrochemical (EC) oxygen intercalation on a 50 micron highly twinned single crystal mounted in a specially designed EC cell using synchrotron diffraction at BM01A@ESRF. We have followed phase transitions (ortho → tetra → ortho) and evolution of domain structure with a very special focus on the presence or absence of grain boundaries. This in-situ study allowed during an EC reaction to explore whole reciprocal space i.e. microstructure, twin domains including diffuse scattering.

KFM 19.4 Wed 16:10 EMH 025

A green magnetic cooling device built using upcycled NdFeB magnets — •Dimitri Benke[1], Jonas Wortmann[1], Marc Pabst[1], Tino Gottschall[2], Iliya Radulov[1], Konstantin Skokov[1], Oliver Gutfleisch[1], Davide Prosperi[3], Peter Afiuny[3], and Miha Zakotnik[3] — [1]TU Darmstadt, Darmstadt, Deutschland — [2]Helmholtz-Zentrum Dresden-Rossendorf, Rossendorf, Deutschland — [3]Urban Mining Company, Austin, USA

Magnetocaloric devices hold the potential to satisfy the rising demand for cooling in the future. One remaining challenge is to reduce the high ecological footprint of the permanent magnets driving the magnetic cooling cycle. Existing devices use neodymium-iron-boron (NdFeB)-type permanent magnets, which account for more than 50% of the ecological footprint of the appliance. To overcome this hurdle, TU Darmstadt and Urban Mining Company have built the first working magnetocaloric device that uses recycled NdFeB as a magnetic field source. Coupling this with optimisation of the magnets and their geometry, it is possible to further reduce the ecological footprint. Together, these two approaches help to position magnetic cooling as a realistic and sustainable cooling technology.

20 min. break

KFM 19.5 Wed 16:50 EMH 025

Electromagnetic Functionalization of Wide Band Gap Dielectric Oxides by Interstitial Doping — •Dae-Sung Park[1,3], Haiyuan Wang[2], Diana Rata[3], Akash Bhatnagar[1,3], Igor Maznichenko[3], Sergey Ostanin[3], and Kathrin Dörr[3] — [1]Zentrum für Innovationskompetenz SiLi-nano, Halle, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [3]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

In solid-state oxides, methods such as chemical doping/alloying, mechanical strain, defect engineering, and integration of distinct materials, have been conventionally used to modify a wide range of physical and chemical properties. Here, we demonstrate an extraordinary interstitial doping effect centred around a light element (boron) cation. The host matrix is a novel composite system synthesised from discrete bulk LaAlO3:LaBO3 compounds. Our results show a spontaneous ordering of the interstitial boron cations within the host LaAlO3 lattices, and subsequent effective spin-polarized charge injection into the neighbouring cations. These ordered interstitials lead to a series of remarkable functional properties, namely, cation-dominated electrical switching and ferromagnetism. Therefore, interstitial boron doping serves to transform a wide band gap and non-magnetic dielectric bulk oxide into a high-temperature ferromagnetic ionic-electronic conductor. This interstitial doping effect is proposed to be a general route for tailoring new multifunctional properties in bulk oxides for smart materials applications such as non-volatile information and spintronic devices.

KFM 19.6 Wed 17:10 EMH 025

The impact of different Si surface terminations in the (001) n-Si/NiOx heterojunction on the oxygen evolution reaction (OER) by XPS and electrochemical methods — •Sven Tengeler, Mathias Fingerle, Wolfram Calvet, Céline Steinert, Bernhard Kaiser, Thomas Mayer, and Wolfram Jaegermann — Technische Universität Darmstadt

The interaction between (001) n-Si and NiOx was investigated with regard to the oxygen evolution reaction (OER), applicable either for

water splitting or CO2 reduction. Thin layers of NiOx were deposited step by step by reactive sputter deposition and analyzed in-situ after each step using X-ray photoelectron spectroscopy (XPS) for Si with different surface preparations: H-termination, thermally grown oxide (2 Å) and native oxide (4 Å). Upon contact formation the initial flat band like situation in the Si substrates changed to a 0.35-0.4 eV upward band bending for all three heterojunctions, hole extraction barriers are low.

The observed similarities in the heterojunctions should result in the same similarities for the OER performance. However, cyclic voltammetry measurements reveal a shift of more than 0,2 V in dependence of the surface treatment. Using chopped light measurements, this underperformance could be attributed to a higher density of defect states at the Si surface. Apparently a 4 Å SiO2 layer is sufficient protection to prevent the formation of defect states during NiOx deposition, thinner protective layers or none at all result in increased defect states, while thicker layers perform poorly due to their high ohmic resistance.

KFM 19.7 Wed 17:30 EMH 025

Interaction of water with wet-chemically etched p-GaInP2(100) surface — Andreas Hajduk[1], •Mikhail Lebedev[2], Bernhard Kaiser[1], and Wolfram Jaegermann[1] — [1]TU Darmstadt, AG Oberflächenforschung, Otto-Berndt-Straße 3, 64287 Darmstadt — [2]Ioffe Institute, Politekhnicheskaya 26, St. Petersburg, 194021 Russia

Photoelectrochemical water splitting offers the possibility to convert solar energy directly into a chemical fuel and therefore is a promising candidate for a sustainable energy solution in the future. GaInP2 with a direct bandgap of 1.8-1.9 eV shows so far the highest reported solar-to-hydrogen conversion efficiencies. Nevertheless, the fast photocorrosion of III-V semiconductors in aqueous solution presents a major obstacle for their use as efficient and stable photoelectrodes. Interaction of water with chemically etched p-GaInP2(100) surface covered with a submonolayer of residual oxides is studied by synchrotron photoemission spectroscopy to gain insight into the solid/solvent interaction at the semiconductor/electrolyte interface. Photoemission spectra obtained after emersion of the semiconductor from liquid water at room temperature and adsorption of H2O molecules at liquid-nitrogen temperature are compared to understand the chemistry of the GaInP2(100)/H2O interface. Valence band spectra indicate dissociative adsorption of water molecules both after emersion and after adsorption experiments. Surface-sensitive core level spectra reveal the interaction of H2O molecules with surface phosphorous and gallium atoms.

KFM 20: Multiferroic Oxide Thin Films and Heterostructures II (joint session KFM/TT/MA)

Organizers: César Magén - University of Zaragoza, Aragón (Spain); Kathrin Dörr - Martin-Luther-Universität Halle-Wittenberg - Halle

Time: Wednesday 15:00–18:15 Location: EMH 225

Invited Talk KFM 20.1 Wed 15:00 EMH 225

Merging Nonlinear Optics and Multiferroic Heterostructure Design — •Manfred Fiebig — Department of Materials, ETH Zurich, Vladimir-Prelog-Weg 4, 8093 Zurich, Switzerland

Despite the large variety of valuable tools that are at our disposals for characterizing oxide thin films, some of their functionalities remain invisible. Buried layers and their ordering and interactions are difficult to access. We show how optical second harmonic generation (SHG) allows us to detect such hidden properties. We show how the real-time dynamics of a domain patterns in multiferroic $BiFeO_3$ is tracked by SHG through a ferromagnetic metallic cover layer, thus identify the magnetoelectric domain coupling nondestructively during the poling process [1]. SHG furthermore resolves the domain-wall architecture in tetragonal ferroelectric thin films. In $PbZr_{0.2}Ti_{0.8}O_3$ films it quantifies the buried distribution of a- and c-domains and reveals that c-domain walls exhibit a mixed Ising-Néel-type transverse rotation of polarization across the wall [2]. Finally, by coupling a laser beam into the deposition chamber, SHG follows the evolution of the spontaneous polarization of complex multiferroic heterostructure in real time and with monolayer sensitivity throughout the entire deposition process. Such in-situ SHG allows us tailor heterostructures with an arbitrary sequence of ordered states which could become the key to whole new class of functional ferroelectric materials [3].

[1] M. Trassin *et al.*, Adv. Mater. **27**, 4871 (2015). **[2]** G. De Luca*et al.*, M. Trassin, Adv. Mater. **29**, 1605145 (2017). **[3]** G. De Luca*et al.*, Nature Comm. **8**, 1419 (2017)

KFM 20.2 Wed 15:30 EMH 225

Real-time observation of polarization emergence in ultrathin ferroelectric heterostructures — •Gabriele De Luca[1], Nives Bonacic[1], Johanna Nordlander[1], Corinne Bouillet[2], Manfred Fiebig[1], and Morgan Trassin[1] — [1]Department of Materials, ETH Zurich, Vladimir-Prelog-Weg 4, 8093, Zurich, Switzerland — [2]Institut de Physique et Chimie des Matériaux de Strasbourg CNRS UMR 7504, 67034, Strasbourg, France

The integration of functional properties into oxide multilayer architectures demands for atomic precision. In-situ diagnostic tools guarantee high structural quality but are usually insensitive to the functionality targeted with the actual deposition. The conventional optimization process requires multiple samples and ex-situ analysis. Here, we take advantage of the non-invasive nature of optical probes and monitor the functionality during growth. Taking ferroelectricity as a representative case, we show that optical in-situ second harmonic generation (ISHG) analysis can be performed simultaneous to the pulsed-laser-deposition growth operation. We follow the evolution of the spontaneous polarization in real time and with monolayer resolution throughout the deposition process [1]. Such direct access allows validating the growth of oxide heterostructures with an arbitrary sequence of up- and down-polarized ferroelectric layers. This is only the first step in the implementation of ISHG as a growth diagnostic tool. The in-situ access to emerging properties enables an unprecedented degree of control that can promote the engineering of oxides functionalities to a completely new level.

[1] G. De Luca et al., Nat. Commun. 8, 1419 (2017)

KFM 20.3 Wed 15:45 EMH 225

Controlling the effect of the depolarizing field in $BaTiO_3$-$SrTiO_3$ multilayers — •Nives Bonacic[1], Gabriele De Luca[1], Shovon Pal[1], Marco Campanini[2], Marta D. Rossell[2], Morgan Trassin[1], and Manfred Fiebig[1] — [1]ETH Zurich, Department of Materials — [2]EMPA, Switzerland

The demand for ever-smaller devices has been approaching the fundamental limits of ultrathin ferroelectric films. In the low-thickness regime, maintaining a large, stable and switchable ferroelectric polarization relies on the control of the strain state, thickness, interface termination and electrostatic conditions. Achieving a robust polarization or a controlled domain state remains, however, challenging. Imperfect charge screening at interfaces results in non-cancellation of internal fields that can in extreme case annihilate ferroelectricity. Taking ($BaTiO_3$-$SrRuO_3$) capacitor-like heterostructures as a model system, we directly access the polarization and the domain state during the film deposition using optical second harmonic generation [1]. We observe a previously elusive impact of the evolving electrostatic environment on the $BaTiO_3$ domain state simultaneously with the growth. The initial phase of the top-electrode deposition is accompanied by temporary enhancement of built-in fields in the ferroelectric layer resulting in 180° domain formation. We discuss ways to manipulate the depolarizing field and control the polarization during the growth as it presents a possible route towards a novel class of oxide-electronic devices. [1] G. De Luca et al., Nat. Commun. 1419 (2017).

KFM 20.4 Wed 16:00 EMH 225

In-situ characterization of improper ferroelectricity in ultrathin multiferroic h-$YMnO_3$ films — •Johanna Nordlander[1], Marta D. Rossell[2], Rolf Erni[2], Manfred Fiebig[1], and Morgan Trassin[1] — [1]ETH, Zürich, Switzerland — [2]EMPA, Dübendorf, Switzerland

Improper ferroelectrics are materials whose ferroelectricity is driven by

another, primary, order parameter. This type of ferroelectricity can lead to exotic properties that do not exist in standard ferroelectrics. In the case of bulk hexagonal manganites, the structural trimerization results in a topologically protected vortex domain structure. Due to their potential for extending existing technological applications with complex functional properties, there has been a revival of interest in hexagonal manganite thin films. Here we demonstrate the growth of highly oriented, epitaxial hexagonal $YMnO_3$ thin films using pulsed laser deposition. We use in-situ optical second harmonic generation (SHG) to non-invasively probe, in real time during and after the deposition process, the ferroic state of the films in the ultrathin regime. With the complementary use of reflection high-energy electron diffraction (RHEED), the emerging polarization of $YMnO_3$ is resolved with monolayer precision. The characteristic improper ferroelectric domain pattern in the ultrathin $YMnO_3$ films is investigated using scanning transmission electron microscopy. This work provides new insights in the early stage of improper ferroelectricity and domain state in hexagonal $YMnO_3$ thin films - especially the drastic influence of epitaxial strain and reduced dimensions on the ferroelectric Curie temperature.

KFM 20.5 Wed 16:15 EMH 225

Multiferroic and magnetoelectric nanocomposites for data processing — •Wolfgang Kleemann — Physics Department, University Duisburg-Esssen, 47048 Duisburg, Germany

Switching of magnetism with electric fields and magnetic control of electric polarization are challenging tasks for multiferroic and magnetoelectric materials. Various composite realizations appear most promising for data processing applications: (1) We propose 2-2 nanocomposites based on magnetoelectric (ME) chromia (111) films (Cr2O3), which allow electric switching of the magnetization of epitaxially grown ultrathin ferromagnetic Co/Pt/Co trilayers via interfacial exchange bias. Random access memory (MERAM) and logic cell MEXOR have been approved [1]. (2) Regular 2-1 composites of magnetostrictive cobalt ferrite (CoFe2O4) nanopillars are PLD-grown in a piezoelectric film of barium titanate (BaTiO3). In a transverse magnetic field they exert a staggered shear stress-induced surface polarization pattern in the BaTiO3 environment [2]. Possible data storage applications will be discussed. (3) Ceramic 0-3 composites of antiferromagnetic-ferroelectric Bi(Fe,Co)O3 nanoclusters embedded in K0.5Bi0.5TiO3 reveal giant linear magneto-electric response via bilinear piezo-magneto-electric coupling, M = αE with α = 10-5 s/m [3]. They are candidates for future electrically addressable nanodot mass memory devices. [1] US Pat. 7,719,883 B2 (2010). [2] Nature Comm. 4, 2051 (2013). [3] Adv. Funct. Mater. 26, 2111 (2016).

15 min. break

KFM 20.6 Wed 17:00 EMH 225

Local observables in inhomogenous systems — •Raffaele Resta[1] and Antimo Marrazzo[2] — [1]IOM-CNR, Trieste, Italy — [2]THEOS, EPF Lausanne, Switzerland

When addressing inhomogenous systems (e.g. heterostructures) a key issue is which physical properties do (or do not) admit a local expression. It is known since long time that spin magnetization is indeed local, and that the density of spin magnetization is well defined quantity. It is also known (since the early 1990s) that instead polarization density is an ill defined concept. Bulk electric polarization P is a Berry phase of the electronic wavefunction: as such it does not admit any local representation. In analogy with P, orbital magnetization is a geometrical property of the electronic ground state; but at variance with P, it also admits a local representation with a well defined density in coordinate space [1,2]. Here we address one further property: the insulating/metallic character of a region in an inhomogeneous system. A well known tool to investigate this property is the local density of states, but it is not a ground-state property. According to Kohn (1964) the insulating/metallic character of a material stems from a different organization of the electrons in their ground state. We define a local "marker" which probes such organization, and we validate it by means of computer simulations.

[1] R. Bianco and R. Resta, Phys. Rev. Lett. 110, 087202 (2013)
[2] A. Marrazzo and R. Resta, Phys. Rev. Lett. 116, 137201 (2016)

KFM 20.7 Wed 17:15 EMH 225

Magnetoelectric coupling and multicaloric effects in $SrMnO_3$ — Alexander Edström and •Claude Ederer — Materials Theory, ETH Zürich, Switzerland

$SrMnO_3$ is a G-type antiferromagnet where ferroelectricity can be induced by epitaxial strain or Ba-substitution. Furthermore, a transition to ferromagnetic order has been predicted under large tensile strain [1], and the two ordering temperatures can in principle be tuned to coincide by varying both strain and composition. $SrMnO_3$ is thus a very rare example of a multiferroic with proper ferroelectric and magnetic order and similar ordering temperatures.

We use first principles electronic structure calculations in combination with first-principles-derived effective model Hamiltonians to obtain the temperature and strain-dependent ferroelectric/magnetic phase diagram of $SrMnO_3$. We then explore coupling effects between the polar and magnetic order. A particular focus thereby are possible multi-caloric effects, i.e., adiabatic temperature changes induced by applied electric and/or magnetic fields, that are very promising for future solid state cooling devices [2].

[1] J. H. Lee and K. M. Rabe, Phys. Rev. Lett. 104, 207204 (2010).
[2] X. Moya, S. Kar-Narayan, and N. D. Mathur, Nature Mater. 13, 439 (2014).

KFM 20.8 Wed 17:30 EMH 225

Octahedral tilting, phonons and Goldstone modes in 111-strained perovskites — Magnus Moreau[1], Astrid Marthinsen[1], Sinead Majella Griffin[2], Tor Grande[1], Thomas Tybell[1], and •Sverre Magnus Selbach[1] — [1]NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]Lawrence Berkeley National Laboratory, Berkeley, California, USA

Epitaxial strain has been extensively explored to enhance existing and enable new functional properties in perovskites oxide thin films, with the majority of the work done on 001-oriented films. Recent advances in film growth has made other epitaxial orientations possible, and particularly 111-oriented films show interesting properties because of the different symmetry and chemical bonding at the terminating (111) facet. We use density functional theory (DFT) calculations to study the different response to 111- and 001-strain of the octahedral tilt system and the crystal field splitting of perovskite oxides. Unlike 001-strain, 111-strain is parallel to the edges of the oxygen octahedra, and tensile 111-strain can emulate negative hydrostatic pressure, which is not easily realised experimentally for bulk materials. General trends for how 111-strain affects polar and rotational modes are outlined based on calculations of twenty common perovskites. Furthermore, we show that in SrMnO3 compressive 111-strain give rise to Goldstone-like phonon modes with a Mexican hat-shaped energy surface, while large tensile strain can induce polar Goldstone modes. The chemical and structural requirements for engineering structural Goldstone modes in 111-strained perovskites are finally discussed.

KFM 20.9 Wed 17:45 EMH 225

Voltage controlled magnetization dynamics in nanostructured multiferroic multilayer systems — •Alexander F. Schäffer and Jamal Berakdar — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany

We investigate the control of magnetization dynamics by applying localized voltages in the framework of nanostructured multiferroic heterostructures. Manipulations of the magnetic anisotropy are spatially controlled by nanostructuring. This combination is utilized as a toolbox to excite or manipulate magnetic systems in order to manipulate multiple magnetic phenomena, such as the magnon dispersion, local spin current sources, or local non-collinear magnetic textures. Full-fledged numerical calculations for realistic systems along with basic analytical models will be shown in order to point towards opportunities for further experimental investigations and applications.

KFM 20.10 Wed 18:00 EMH 225

Electronic and magnetic properties of $BaFeO_3$-Pt(111) in a quasicrystalline approximant structure — •Waheed A. Adeagbo, Igor V. Maznichenko, Hichem Ben-Hamed, Ingrid Mertig, and Wolfram Hergert — Institute of Physics, Martin Luther University Halle-Wittenberg, Germany

The first reported formation of an oxidic quasicrystal (OQC) $BaTiO_3$ (BTO) on Pt(111) has led to finding of other quasicrystalline (QC) perovskites like $SrTiO_3$ on the same substrate. Since these are non-magnetic, it is interesting to investigate the properties of magnetic perovskites in corresponding approximant structures. $BaFeO_3$ (BFO) has a very good lattice match with Pt(111) and also a robust magnetic properties which could add new interesting features to the QC systems. In this work we have carried out first principles study on the periodic BFO bulk crystals properties in the cubic (c-BFO) and the

hexagonal (6*h*-BFO) phases. The derived OQC thin film which exhibits strong similarities to the BTO-derived OQC with respect to the local tiling geometry of Kepler's approximant was also studied both in the free standing and in the supported phase on Pt(111) surface. Our results shows that the anti-ferromagnetic 6*h*-BFO bulk phase is preferable ground state to *c*-BFO phase. Like in BTO-OQC approximant, the BFO also shows all four Fe atoms surrounded by three O atoms with the FeO_3 units separated by Barium atoms with the total stoichiometry $Ba_5Fe_4O_{10}$. Since the exact oxidation states of the Fe and the role of O vacancy in the stabilization is unknown for these systems, the results of these will be presented together with the magnetic contribution.

KFM 21: Lithography II: Focused Electron Beam Induced Processing: 3D Nano-Printing for Material Science (Focussed Session): Afternoon Session (joint session DS/KFM)

Considering 3D printing using fused-deposition modeling or higher-resolution variants with lasers applicable to polymers and metals, an analogous approach exists on the nanometer scale. With the aid of focused electron beam-induced deposition (FEBID) it is possible to create solid-state structures on the nanoscale. However, in contradistinction to large-scale 3D printing of simple plastic or metallic structures, FEBID is able to directly provide nano-materials with a wealth of interesting electronic, optical and magnetic properties. Due to this, focused electron beam-induced deposition has experienced a rapid expansion in the breadth of its application fields over the last 10 years. FEBID uses precursor gases which, being adsorbed on a surface, are dissociated in the focussed electron beam to form the deposit. Intensive research has pushed the capabilities of FEBID in two important areas. It is now possible to obtain fully metallic nanostructures of Fe, Co and FeCo-alloys and also of Au and Pt. In addition, very recently the simulation-guided nano-manufacturing of 3D structures has matured to such a degree that even complex 3D objects can now be fabricated under controlled conditions. The focused session will address these new developments spanning the range from the fundamentals of electron-precursor interaction, covering aspects of the rational design of optimized precursors, and showing recent work on superconducting, magnetic and plasmonically active materials, both in 2D and 3D.

Organized by

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Name: Dr. Ivo Utke, Institution: EMPA, Swiss Laboratories for Materials Science and Technology, City: Thun, Country: Switzerland, Email: Ivo.Utke@empa.ch, Telephone number: +41-58-765-6257

Time: Wednesday 15:00–18:00 Location: H 2032

KFM 21.1 Wed 15:00 H 2032

FEBIP on Metal-Organic Frameworks — •Christian Preischl[1], Elif Bilgilisoy[1], Florian Vollnhals[1], Kai Ahlenhof[2], Petra Swiderek[2], Hartmut Gliemann[3], Christof Wöll[3], and Hubertus Marbach[1] — [1]Physik. Chemie II, FAU Erlangen — [2]IAPC, Universität Bremen — [3]Institut f. funktionelle Grenzflächen, KIT

We report the fabrication of nanostructures down to single digit nanometer scale on metal-organic frameworks (MOFs) by FEBIP. Next to EBID[1], our second technique is Electron Beam Induced Surface Activation (EBISA). In EBISA the surface is locally activated by an electron beam and the subsequently dosed precursor is catalytically decomposed at the activated sites and forms a deposit.[2] Both approaches were investigated with $Fe(CO)_5$ and $Co(CO)_3NO$ on HKUST-1 and Cu-oxalate which is somewhat similar to HKUST-1 but the benzylic part in the organic linker is missing compared to the latter. Both samples were grown in a layer-by-layer method.[3][4] We demonstrate that both precursors are suitable for EBID on both samples, whereas EBISA works only with $Fe(CO)_5$ on the HKUST-1. We will compare the corresponding results and discuss especially the high potential of MOFs as substrates for novel FEBIP processes towards the fabrication 3D materials.

[1] W. van Dorp, C.W. Hagen, J. Appl. Phys. 104 (2008), 081301 [2] H. Marbach, Appl. Phys. A 117 (2014), 987; Drost et al., Small Methods 1 (2017), 1700095 [3] O. Shekhah et al., Angew. Chem. Int. Ed. 48 (2009), 5038 [4] I. Schrader et al., Langmuir 30 (2014), 11945

KFM 21.2 Wed 15:15 H 2032

Focused Electron Beam Induced Deposition with halogenated organometallic Ru compounds — •Jakub Jurczyk[1,2], Christopher Brewer[3], Olivia Hawkins[3], Czeslaw Kapusta[2], Lisa McElwee-White[3], and Ivo Utke[1] — [1]Empa - Swiss Federal Laboratories for Materials Science and Technology,Thun, Switzerland — [2]AGH University of Science and Technology in Krakow, Kraków, Poland — [3]University of Florida, Gainesville, USA

Focused Electron Beam Induced Deposition (FEBID) studies of potential organometallic halogenated ruthenium precursors were performed. By now the best Ru FEBID result was achieved using bis(ethylcyclopentyldienyl) ruthenium(II) [1] giving a C:Ru ratio of 9:1 (10 at.% Ru) in as deposited material. Recent gas phase [2] and surface science studies [3] selected halogenated organometallic compounds as potential FEBID precursors. In this contribution we present three of them: n-allyl-Ru(CO)3Cl, n-allyl-Ru(CO)3Br, n-allyl-Ru(CO)3I. The deposit metal content was investigated as function of growth regimes and writing strategies for vertical and planar structures. First promising results of up to 20 at.% of Ru in as deposited material were achieved. Electrical properties of as deposited and annealed nanowires will be presented.

[1] J.H. Noh et al., App. Phys. A, 117, (2014), 1705-1713 [2] R. M. Thorman et al., Phys. Chem. Chem. Phys, 19, (2017), 13264-13271 [3] Spencer et al., J. Phys. Chem. C, 119, (2015), 15349-15359

KFM 21.3 Wed 15:30 H 2032

Electron-induced reactions of surface-grown metal organic layers — •Kai Ahlenhoff and Petra Swiderek — University of Bremen, Institute for Applied and Physical Chemistry, Bremen, Germany

Metal-containing coordination materials grown on surfaces using layer-by-layer self-assembly processes are advantageous for focused electron beam deposition (FEBID) processes for several reasons. First, multi-

layer materials can serve as precursors which enable high processing speed due to their large surface density [1]. Also, an adlayer on a substrate used in a regular FEBID process relying on volatile precursors can suppress secondary electron emission from the underlying solid and thus lead to more precisely defined deposit shapes [2]. Third, the layer may be activated by an electron beam to provide a template for area-selective autocatalytic deposit growth in an EBISA process [2].

Despite these advantages, little is known about the electron-induced reactions in such materials and the resulting products. Therefore, this contribution presents studies on electron-induced desorption (ESD) from and post-irradiation reflection absorption infrared spectroscopy (RAIRS) of several surface grown metal-organic coordination polymers such as copper(II)oxalate [3] and HKUST-1 [4] but also including novel FEBID precursors.

References: [1] M. Bresin et al. Nanotechnol. 24 (2013) 035301. [2] M. Drost et al., SMALL Methods 1 (2017) 1700095. [3] K. Rückriem et al., Beilstein J. Nanotechnol. 7 (2016) 852. [4] B.W. Jacobs et al., Nanotechnol. 22 (2011) 375601.

KFM 21.4 Wed 15:45 H 2032

Tuning and in-situ monitoring the hall resistance of ferromagnetic FEBID structures — •Roland Sachser and Michael Huth — Physikalisches Institut, Goethe-University, Frankfurt am Main, Germany

$HFeCo_3(CO)_{12}$ is an excellent FEBID precursor, which allows the deposition of magnetic and metallic CoFe alloy nanostructures. In contrast, the widely used $(CH_3)_3CH_3C_5H_4Pt$ standard precursor results in insulating deposits, consisting of Pt nanograins embedded in a carbonaceous matrix. In this contribution we will present measurements on samples prepared via co-deposition of both precursors. Varying the deposition conditions, the metal content of the deposits, and thus, the resistivity and the Hall resistance of the samples can be tuned. Furthermore, the co-deposited samples are sensitive to post-growth electron beam irradiation, which influences its electrical transport properties, as it is already known for normal FEBID deposits obtained by the Pt-precursor. We will show in-situ measurements of the Hall resistance directly inside the SEM by using the magnetic field provided by the immersion lens of the instrument. Further characterization is done via temperature-dependent electrical and magnetotransport measurements.

KFM 21.5 Wed 16:00 H 2032

Purified and crystalline three-dimensional electron-beam-induced deposits: the successful case of cobalt — Javier Pablo-Navarro[1], César Magén[1,2], and •José María De Teresa[1,2] — [1]Laboratorio de Microscopías Avanzadas (LMA) - Instituto de Nanociencia de Aragón (INA), Universidad de Zaragoza, 50018 Zaragoza, Spain. — [2]Instituto de Ciencia de Materiales de Aragón (ICMA), Universidad de Zaragoza-CSIC, 50009 Zaragoza, Spain.

Purified and crystalline 3D cobalt nanowires of diameter below 90 nm have been fabricated by ex-situ high-vacuum annealing at 600 Celsius degrees after FEBID growth. While increasing the metallic content of the nanowires up to 95 atomic percent, the thermal annealing process induces the recrystallization of the pseudo-amorphous as-grown structure into bulk-like, hcp and fcc crystallites with lateral sizes comparable to the width of the nanowire. The net magnetization increases 80 percent with respect to as-grown values, close to the bulk cobalt value. This achievement opens new pathways for applications of this synthetic method in the fabrication of either individual or arrays of 3D high-purity and crystalline cobalt nanowires for high-density memory and logic devices, nanosensors and actuators, and could be a viable method to obtain other pure and crystalline 3D materials by FEBID.

KFM 21.6 Wed 16:15 H 2032

Exploring new copper complexes for FEBID — •Luisa Berger[1], Katarzyna Madajska[2], Nils Boysen[3], Iwona Barbara Szymánska[2], Anjana Devi[3], and Ivo Utke[1] — [1]Empa - Swiss Federal Laboratories for Materials Science and Technology, Thun, Switzerland — [2]Nicolaus Copernicus University, Torun, Poland — [3]Ruhr-Universität Bochum, Germany

Focused electron beam induced deposition (FEBID) is a well-established maskless direct write method for nanostructures [1]. The deposition of pure copper with FEBID has not been achieved so far and metal contents typically reached 13-25 at.% [2]. By exploring novel copper precursor classes - fluorinated copper carboxylates ([Cu2(u-O2CC2F5)4], [Cu2(EtNH2)2(u-O2CC2F5)4]) and a fluorine-free β-diketonate (Cu(tbaoac)2) - we intend to achieve the deposition of high purity structures. The latter was employed in FEBID recently [3] while carboxylates were reported as CVD precursors [4]. The influence of varying deposition parameters on appearance and composition was investigated. First interesting results lead to copper contents of 25 at.%.

[1] I. Utke, A. Gölzhäuser, Angew. Chem. Int. Ed. 49 (2010), 9328.
[2] A. Luisier et al., Journal of The Electrochemical Society, 151 (2004) C535.
[3] C. Haverkamp, K. Höflich et al., Beilstein Journal of Nanotechnology 2017 (in review)
[4] P. Piszczek, I. B. Szymańska, Chem. Vap. Deposition, 19 (2013) 251.

15 min. break.

KFM 21.7 Wed 16:45 H 2032

Dedicated AS-ALD micro-reactor for FEBID nano-templates — •Peter Gruszka, Giorgia Di Prima, Roland Sachser, and Michael Huth — Goethe Universität, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

In recent years, conventional methods of nano-structuring are slowly reaching their lower limits. A novel bottom-up approach emerged[1], which combines focused electron beam induced deposition(FEBID) and area-selective atomic layer deposition(AS-ALD). FEBID is a serial, bottom-up and direct-write technique yielding structures with superior lateral resolution ($<$ 10 nm), but with poor material quality. In contrast, ALD and especially AS-ALD are parallel and bottom-up approaches with exceptional thickness control resulting in high purity sub-nano films.

We successfully performed the combined FEBID-ALD process in our Nova 600 Dual Beam scanning electron microscope.[2] The ALD experiments were conducted on purified platinum FEBID-nanostructures[3] which were monitored via in-situ conductance measurements. For further investigation and optimization, we built a dedicated AS-ALD micro-reactor.

[1] Mackus, et al., J. Appl. Phys 107 (2010), 116102
[2] Di Prima, et al., Nano Futures 1(2) (2017), 25005
[3] Sachser, et al., ACS Appl. Mater. Interfaces 6 (2014), 15868

KFM 21.8 Wed 17:00 H 2032

Fabrication of multi-component nanostructures by FEBID — •Fabrizio Porrati[1], Roland Sachser[1], Sven Barth[2], Gian Carlo Gazzadi[3], Stefano Frabboni[3], Christian Gspan[4], Harald Plank[4], Andreas Terfort[5], and Michael Huth[1] — [1]Goethe-Universität, Institut of Physics, Frankfurt am Main, Germany — [2]TU Vienna, Institute of Materials Chemistry, Wien, Austria — [3]University of Modena and Reggio Emilia, FIM Department, Modena, Italy — [4]TU Graz, Institute for Electron Microscopy and Nanoanalysis, Graz, Austria — [5]Goethe-Universität,Institute for Inorganic and Analytical Chemistry, Frankfurt am Main, Germany

The fabrication of multi-component polycrystalline or granular metals by FEBID represents a challenging research approach for the design of novel nanostructured materials. Currently, there are three different approaches for the fabrication of multi-component FEBID nanostructures: 1. deposition by single source heteronuclear precursors; 2. codeposition using two different precursors; 3. intermixing of multilayer nanostructures fabricated with different precursors by low-energy electron irradiation. These fabrication approaches allow the fabrication of a large number of tunable alloy nanostructured and intermetallic compounds. In this contribution, we present some examples of binary and ternary nanostructures fabricated by following these routes. In particular, we report on the fabrication, the structural characterization and magnetotransport measurements of CoFe alloys and Co2FeSi Heusler compounds.

KFM 21.9 Wed 17:15 H 2032

Ac response of nano-granular metals prepared via FEBID — •Marc Hanefeld and Michael Huth — Physikalisches Institut, Goethe Universität, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

Granular metals are of great interest for material sciences due to their diverse electronic transport properties and can generally be described as metallic nanoparticles surrounded by a dielectric amorphous matrix. They show promising possibilities for applications in different sensing mechanisms [1] and pose a topic of ongoing research concerning their response to a time-dependant ac stimulus [2].

Focused Electron Beam Induced Deposition (FEBID) is a versatile technique to create nano-granular metals comprising a variety of elements and a high tunability of the samples properties. Additionally, electron irradiation is the perfect tool to tune important conduction parameters like the inter-grain coupling strength and the volume fraction of the crystallites compared to the surrounding matrix, ultimately influencing the conductance regime of the deposits. In our group we have a wide knowledge about Pt(C)-FEBID deposits and the effect of electron irradiation upon them, as well as their dc electronic transport properties [1]. We will present first measurements on the ac response of such deposits and show the capabilities of FEBID to create an ideal model environment for an in depth analysis of the ac conduction characteristics of granular metals depending on their properties.
[1] Huth, et al., Microelect. Eng. 2017. doi:10.1016/j.mee.2017.10.012.
[2] Bakkali, et al., Sci. Rep. 2016;6:29676. doi:10.1038/srep29676.

KFM 21.10 Wed 17:30 H 2032

Energy collection from green-house infra-red emission using nanogranular compoundmaterials — •Koops Hans Wilfried Peter — HaWilKo GmbH , Ober-Ramstadt, Germany

According to a 10 years average measurement of NASA of the earth's energy household, the sun sends 340,4 W/m^2 direct to the earth, but only 163,3 W/m^2 reach the ground. In the IR a backreflection from greenhouse gases delivers 340 W/m^2.

A nanogranular Pt/C material has a bandgap of 128 meV, which allows to absorb IR-Light. This radiation can be absorbed by a nanocrystalline Pt/C compound. Large absorber areas can be used. Silicon material absorbes only energies above 1.3 eV during daylight from the visible light. The green house gases, however, emit their radiation all day and night in the IR. The absorbed IR photons can be stored in the compound material as coherent Boson fields. A field gradient applied to such fields can move the Bosons and make them decay at the end of the field, and release electrons as a current. HaWilKo can produce a 1 cm^2 large sheet to demonstrate the energy harvesting in the IR.

KFM 21.11 Wed 17:45 H 2032

Coordination compounds for focused electron beam induced deposition (FEBID) — •Iwona Szymańska. and Katarzyna Madajska — Faculty of Chemistry, Nicolaus Copernicus University in Toruń, Gagarina 7, 87-100 Toruń, Poland

Focused electron beam induced deposition is a direct maskless nanolithography technique. The compounds applied as FEBID precursors should effectively generate volatile metal carriers, which are transported over a substrate. Next, they are irradiated by high-energy electrons and decompose forming nanomaterials [1]. Copper and silver exhibit high electrical and thermal conductivity and are extensively used in microelectronics.

Copper and silver carboxylate compounds were applied as CVD precursors [2,3]. Carboxylates are able to coordinate as monodentates, chelates, and bridges forming complexes of diverse nuclearity. Secondary ligands enable manipulating physicochemical parameters of precursors. Research was focused on the copper(II) and silver(I) carboxylate compounds, which seems to be promising for a FEBID process. The usefulness of a thermal analysis, EI MS spectrometry, and VT IR spectroscopy for the FEBID precursors selection was evaluated. The secondary ligand influence was studied basing on primary amines.
Acknowledgements: The authors wish to thank Nicolaus Copernicus University in Toruń (Statute Research no.103) for a financial support.

References: [1] I. Utke et al., Angewandte Chemie Int. Ed., 49 (2010) 9328; [2] A. Grodzicki et al., Coord. Chem. Rev., 249 (2005) 2232; [3] I.B. Szymańska,, Polyhedron, 65 (2013) 82.

KFM 22: Annual General Meeting of the KFM division

Wednesday,14.03.2018, 18:30 - 19:00, EMH025

Time: Wednesday 18:30–19:00 Location: EMH 025

Duration 30 Minutes

KFM 23: Lithography III: Lithography and Structuring (joint session KFM/DS)

While high-resolution 2D lithography and structuring is relatively mature and also widely applied in industrial processes, work on its 3D variant is mostly focusing on fundamental aspects and process development. At the lower edge of possible 3D feature dimensions, certainly methods such as electron beam induced deposition, non-linear multi-photon-laser lithography and thermal scanning probe lithography techniques are required. This session discusses most of these dedicated 3D methods in detail. For the fabrication of complex 2D and 2.5D patterns, advanced electron beam and X-ray methods are continuously developed further. In addition, new methods such as high resolution Talbot lithography for relatively large areas are already entering industrial maturity. This session also discusses some of the latest developments in this field of binary lithography.

Organizer: Robert Kirchner - Technische Universität Dresden

Time: Thursday 9:30–12:50 Location: EMH 025

Invited Talk KFM 23.1 Thu 9:30 EMH 025

3D Nanoprinting via Focused Electron Beams — •Harald Plank[1,2], Robert Winkler[1,2], Jason Fowlkes[3,4], and Philip Rack[3,4] — [1]Institute for Electron Microscopy and Nanoanalysis Graz University of Technology, 8010 Graz, Austria — [2]Graz Centre for Electron Microscopy, 8010 Graz, Austria — [3]Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — [4]Department of Materials Science and Engineering, University of Tennessee, Knoxville, Tennessee 37996, USA

3D-printing of functional structures has emerged to an important technology in research and development. While being reliable on the micro and sub-micron scale, it becomes very challenging when aiming for nano-sized geometries. Among the very few direct-write techniques on that scale, Focused Electron Beam Induced Deposition is one of the promising candidates as this technology has recently done tremendous steps forward. In particular, this technology allows additive fabrication of complex, freestanding 3D nano-architectures on almost any material and surface morphology, which enables entirely new 3D nano-applications (e.g. plasmonics, artificial spin-ice or nano-probes). The contribution starts with an introduction of FEBID and sheds light on recent progress, which leverages this technology from a scientifically oriented fabrication tool into the status of a reliable and predictable 3D-nanoprinter. In the following, several applications are discussed to demonstrate the new possibilities of this generic fabrication technology. Finally, the talk gives an overview of ongoing activities together with future perspectives beyond current limitations.

KFM 23.2 Thu 10:00 EMH 025

3D printing at the diffraction limit: sample injection for time-resolved serial crystallography — •Michael Heymann — MPI of Biochemistry, Am Klopferspitz 18, 82152 Martinsried

Continuous injection using the Gas Dynamic Virtual Nozzle (GDVN)

is a proven sample delivery method for biological imaging using X-ray free-electron lasers. However, many important aspects of GDVN functionality have yet to be thoroughly understood and/or refined due to fabrication limitations. We report the application of 2-photon polymerization as a form of high-resolution 3D printing to fabricate GDVNs with submicron resolution. This allows rapid prototyping of a wide range of nozzle designs from standard CAD drawings to iteratively optimize crucial dimensions for optimal performance. To understand enzyme catalysis and protein conformational changes at the atomic scale, we pioneered mixing-injectors for time-resolved structural biology to record molecular movies of substrate turn-over. We experimentally validate 3D print accuracy, as well as fluid mixing dynamics using X-ray tomographic imaging. We developed mixing-injectors to mix nanocrystals with substrate and to subsequently deliver them into the X-ray interaction region just milliseconds after mixing. This method can determine the structures of transient states and thereby kinetic mechanisms. In a proof of principle experiment, we could follow the catalytic reaction of the M. tuberculosis β-lactamase with the 3rd generation antibiotic ceftriaxone by time-resolved serial crystallography with millisecond to second time resolution at 2Å spatial resolution.

KFM 23.3 Thu 10:20 EMH 025

Fabrication of superior 2D and 3D nano-devices using NanoFrazor lithography — Colin Rawlings[1], Armin Knoll[2], Felix Holzner[1], and •Zhengming Wu[1] — [1]SwissLitho AG, Zurich, Switzerland — [2]IBM Zurich, Switherland

Thermal scanning probe lithography (t-SPL) has recently entered the lithography market as first true alternative or extension to electron beam lithography (EBL). The first dedicated t-SPL systems, called NanoFrazor, have been installed at research facilities in Europe, America, Asia and Australia by the company SwissLitho.

The application range for this new nanofabrication capability is broad and will be demonstrated with the discussion of a selection of examples. Applications that are enabled by the nm-precise 3D patterning include 3D phase plates and finely tuned coupled Gaussian optical microcavities. Furthermore, 3D shaped nanofluidic confinements have been used to precisely control the movement of nanoparticles and nanowires. The high resolution 2D capability was applied e.g. to shape complex plasmonic structures. Furthermore, several superior nanoelectronic devices will be shown. Such devices are predominantly made from randomly dispersed nanowires or 2D materials. Therefore, they benefit strongly from the unique markerless overlay capability of the NanoFrazor lithography, but also from the fact that actually no charged particle beam is used during lithography, which can often damage sensitive materials. Finally, a few examples are shown, how the heated tips are also used for direct modification of surfaces by triggering of a local phase change or a chemical reaction.

KFM 23.4 Thu 10:40 EMH 025

Innovations in photoresists and photopolymers for 2D / 3D micro and nano fabrication — •Anja Voigt, Christine Schuster, Jan Klein, Arne Schleunitz, and Gabi Grützner — micro resist technology GmbH, Koepenicker Str. 325, 12555 Berlin, Germany

Different methods for the manufacture of high resolution 2D and 3D features require a wide range of material solutions based on innovative photoresists and photopolymers. As a commercial resist supplier, micro resist technology aims at providing such solutions tailored for diverse lithography processes, comprising both materials and technology support. The following highlights will be presented:

E-beam lithography is a versatile patterning method for the generation of high resolution nano-patterns. Combining stepwise greyscale exposure and pattern reflow with a positive tone resist results in greyscale patterns of small dimensions.

Greyscale UV lithography of up to 100 micron thick resist films, either by direct laser writing or by conventional mask aligner exposure and a greyscale mask, can generate very deep greyscale micro-patterns. Both very thick films, and considerably smaller pattern features including sharp tips have been successfully fabricated using this technique.

Laser interference lithography is another method which allows the manufacture of nanoscale patterns * periodic patterns even on very large substrates. Whereas two photon absorption (2PA) allows the generation of real 3D patterns at micro and nanoscale.

The development of photoresist and photopolymer materials tailored to meet the requirements of the specific technologies will be presented.

20 min. break

Invited Talk KFM 23.5 Thu 11:20 EMH 025

Diffractive X-ray Optics for Synchrotrons and Free Electron Lasers - a challenge from the lithographer's point of view — •Christian David — Paul Scherrer Institut, Villigen, Switzerland

X-rays are excellent probes for the investigation of matter using scattering, imaging and spectroscopic techniques, offering high penetration capability, spatial and temporal resolution, along with elemental and chemical sensitivity. Accelerator-based photon sources play a key role in these analytical techniques as they offer beams with unique brilliance.

This presentation will give an overview on developments of x-ray instrumentation and experimental techniques based on diffractive optics. These optical elements are designed for short wavelength radiation ranging from the vacuum ultraviolet to hard x-rays and play a key role in the shaping, direction, and detection for a variety of experiments. The key challenges lie in the fabrication of the diffractive structures by advanced nanolithography techniques, as they need to provide dimensions and placement accuracies down to the nanometer scale.

Many applications of these devices include x-ray imaging techniques. The x-ray optics developed at PSI provide spatial resolution down to the 10 nm range, and are designed exploit phase contrast mechanisms or spectroscopic information. Moreover, recent developments of optics for beam splitting and the manipulation of x-ray wave fronts open up new opportunities for time resolved measurements of ultra-fast processes at x-ray lasers.

KFM 23.6 Thu 11:50 EMH 025

A high contrast multilayer process for electron beam lithography using different developers — •Philip Trempler[1], Frank Heyroth[2], Matthias Schirmer[3], Christian Kaiser[3], Tobias Mai[3], and Georg Schmidt[1,2] — [1]Institut für Physik, Martin-Luther Universität Halle-Wittenberg, 06099 Halle (Saale), Germany — [2]Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther Universität Halle-Wittenberg 06099 Halle (Saale), Germany — [3]ALLRESIST GmbH, Am Biotop 14, 15344 Strausberg, Germany

We have developed a new multilayer resist system for the fabrication of three-dimensional nanostructures in a one-step electron beam exposure. The multilayer resist consists of three layers with different sensitivity and different process chemistry. The sensitivity of the three layers to different respective developers allows a very large controllable undercut in the middle layer. The low sensitivity bottom layer can be patterned in high detail almost independent from the pattern exposed in the two layers on top. At acceleration voltage of 30 kV the resist is ideally suited for the fabrication of for example T-gate structures by lift-off in a high reliability process with a very large process window.

KFM 23.7 Thu 12:10 EMH 025

Fabrication of metal nanostructures with focused X-rays — •Andreas Späth, Florian Vollnhals, Fan Tu, Hubertus Marbach, and Rainer H. Fink — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058, Erlangen, Germany

Focused X-ray beam induced deposition (FXBID) is a novel technique for the fabrication of metallic nanostructures by illuminating gas phase precursors with focused soft X-rays in a zone plate based scanning transmission X-ray microscope (STXM). With this technique we have been able to produce localized Co and Mn nanostructures with growth rates and purity competitive with electron beam induced deposition (EBID) [1,2]. We demonstrate that our approach exhibits significant selectivity with respect to incident photon energy leading to enhanced deposition for resonant excitation of the precursor molecule. This finding opens a new field of photon energy selective deposition from precursor mixtures and deposition from various precursors within one production cycle. The impact of several deposition parameters on the growth rate, such as illumination time and precursor pressure are discussed with respect to a deeper understanding of deposition processes and optimization of the procedure. Furthermore, we discuss routes to the formation of magnetic deposits by in-situ cleaning techniques (e.g., co-dosing of reactive gases or annealing). The project is funded by the BMBF (05K16WED).

[1] A. Späth et al., RSC Advances, 2016, 6, 98344.
[2] F. Tu et al., J. Vac. Sci. Technol. B, 2017, 35(3), 031601.

KFM 23.8 Thu 12:30 EMH 025

Printing Uniform Periodic Structures over Large Areas with Displacement Talbot Lithography — •Harun Solak — EU-

LITHA AG, 5416 Kirchdorf, Switzerland

High-resolution periodic patterns such as linear gratings or two-dimensional arrays are required in many applications. This is especially true in photonics, where optimized interaction of light with periodic nanostructures enables creation of new or higher performance devices such as LEDs, lasers, photovoltaic cells, sensors and LCD screens. In such applications, patterns with periodicity approximately in the 0.1-1micrometer-range need to be printed on device surfaces. Current lithographic methods face significant challenges in terms of technical feasibility or cost in meeting the requirements. The recently introduced Displacement Talbot Lithography (DTL) method allows uniform printing of periodic patterns in a non-contact, proximity scheme [1]. The technique enables patterning on non-flat surfaces and in thick photoresist films up to the highest resolution possible at a given exposure wavelength. Photolithography systems specially designed to perform DTL exposures are now available and they find increasing use in various academic and industrial applications [2-3]. The capabilities of this new tool will be introduced with examples of applications. 1. H. Solak, C. Dais, F. Clube, Optics Express, Vol. 19, p. 10866 (2011). 2. H. Le-The, et al, Adv. Mater. Technol. 2017, 2, 1600238. 3. P. M. Coulon, et al Phys. Status Solidi B, 1700445.

KFM 24: Spectroscopy and Microscopy II with Positrons

Chair: Andreas Wagner (Helmholtz-Zentrum Dresden-Rossendorf)

Time: Thursday 9:30–12:20 Location: E 124

Invited Talk KFM 24.1 Thu 9:30 E 124

Discovering Ancient Secrets in Aluminum Alloys – A New Combination of Analytical Techniques and ab-initio Calculations — •Torsten E.M. Staab, Danny Petschke, Frank Lotter, and Elischa Bläss — LCTM, Universität Würzburg, Röntgenring 11, D-97070 Würzburg

Even though Aluminum alloy systems containing only two alloying elements seem to be just textbook example, there are still after decades of research unsolved problems in understanding the earliest stages of the formation of precipitates immediately after solution heat treatment and quenching. We tried to tackle these problems by a combination of different analytic method (DSC, XAFS, SAXS, PALS) combined with ab-initio calculations (SIESTA) of atomic configurations providing atomic positions for calculations of spectroscopic data and, thus, being able to directly compare our calculations to performed experiments.

For AlCu-alloys containing, on the one hand, Mg as a second alloying element we find that Mg-atoms are not catching quenched-in vacancies better than copper, as believe since long ago. However, the precipitation process seems to be triggered by large lattice distortions due to precipitation of Cu-platelets, where Mg atoms prefer lattice sites being under strain. On the other hand, we have been investigating the effect of trace elements in concentrations of 50 - 250ppm in 5N5 purity AlCu, where some of them (In, Sn) are known to bind quenched-in vacancies while other (Pb, Bi) – even larger in size – obviously do not have the same effect. The reason for this behavior is still under discussion.

KFM 24.2 Thu 10:00 E 124

Positron Annihilation Studies using a Superconducting Electron LINAC — •Andreas Wagner[1], Maik Butterling[1], Eric Hirschmann[1], Reinhard Krause-Rehberg[2], Maciej Oskar Liedke[1], and Kay Potzger[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstr. 400, 01328 Dresden, Germany — [2]Martin-Luther-Universität Halle, Institut für Physik, 06099 Halle, Germany

The Helmholtz-Center at Dresden-Rossendorf operates several user beamlines for materials research using positron annihilation energy and lifetime spectroscopy. Two beamlines are being operated at a superconducting electron linear accelerator producing hard X-rays from electron-bremsstrahlung and in turn generating positrons from pair production. While one of the sources uses bremsstrahlung to directly generate positrons inside the sample of interest (named GiPS for Gamma-induced Positron Source), in the second source monoenergetic positrons (named MePS) with energies ranging from 500 eV to 25 keV are used for thin-film studies of porosity and defect studies. Examples of recent experimental results at all facilities will be presented. The MePS facility has partly been funded by the Federal Ministry of Education and Research (BMBF) with the grant PosiAnalyse (05K2013). The initial AIDA system was funded by the Impulse- und Networking fund of the Helmholtz-Association (FKZ VH-VI-442 Memriox). The AIDA facility was funded through the Helmholtz Energy Materials Characterization Platform.

KFM 24.3 Thu 10:20 E 124

An atomic investigation of the clustering on a Friction-Stir-Welding simulated Al-Cu-Li(-Mg) alloy by Positron Annihilation, SAXS, XAFS and DSC — •Danny Petschke, Frank Lotter, and Torsten Staab — University Würzburg, Dep. of Chemistry, Röntgenring 11, D-97070 Würzburg

Al-Cu-Li(-Mg) alloys find wide applications in aviation and aerospace technology due to the reduction of weight and their high strength at the same time. After rolling sheets of these alloys, a defined heat treatment leads to the formation of mainly T1-precipitates. These precipitates are highly efficient in blocking dislocations. When these sheets are joined by Friction-Stir-Welding (FSW), temperatures occuring in the Weld-Nugget (WN) are close to the material's solution treatment temperature. Hence, the T1-precipitates are completely dissolved in this region, which results in a significant hardness-drop. Only sub-nanometer sized GP(B)-zones and CuMg-clusters are formed directly after welding by diffusion processes not understood in detail, yet. We followed the precipitation directly after welding with Differential Scanning Calorimetry (DSC), giving information on formed precipitates, Small Angle X-ray Scattering (SAXS), giving information on size and volume fraction, Positron Annihilation Lifetime Spectroscopy (PALS), being sensitive to the formation and growth of precipitates, and, X-ray absorption spectroscopy (XAFS) as a fingerprint-method to identify the atomic structure by comparing the experimentally obtained spectra to simulations. Therefore, a Welding-Simulator was developed to reproduce the temperature in the welded material.

KFM 24.4 Thu 10:40 E 124

Thermal vacancies in highly diluted Al-In alloy — •Mohamed Elsayed[1,2] and Reinhard Krause-Rehberg[1] — [1]Institut für Physik, Martin-Luther Universität, Halle — [2]Physics Department, Minia University, Egypt

Positron annihilation lifetime spectroscopy (PALS) is applied to study the point defects generated in aluminum indium alloy upon quenching. Al alloy having 0.005-0.025 at % In is used in this study. The samples were homogenized for 2 h in the temperature range 320-620 °C, then rapidly quenched in ice water. They were immediately measured at room temperature (RT) by positron lifetime spectroscopy. The samples were isochronally annealed in the temperature range up to 327 °C in steps of 10 °C, they cooled down after each annealing step to RT and measured by PALS. It is found that the average positron lifetime increases to 240 ps with increasing quenching temperature up to 470 °C and it decreases slightly with further increase of the quenching temperature. A reference pure aluminum (99.9995) samples is quenched at different temperature to show the influence of the alloying element (In) on the vacancy formation. An average lifetime of 170, very close to the bulk value (158 ps), is obtained, indicating the role played by In on the vacancy formation. A defect-related lifetime of 247 ps is obtained in all quenched samples immediately after quenching. This lifetime corresponds mostly to vacancy-In complexes. The defect-related lifetime is found to decrease with increasing annealing temperature up to 127 °C reaching 225 ps, then it increases reaching 280 ps, corresponding to divacancy.

20 min. break

KFM 24.5 Thu 11:20 E 124

Curing processes in ultra low-k materials by positron annihilation spectroscopy — •Maciej Oskar Liedke[1], Nicole Köhler[2], Maik Butterling[1], Eric Hirschmann[1], Ahmed G. Attallah[3], Reinhard Krause-Rehberg[3], Stefan E. Schulz[2,4],

and Andreas Wagner[1] — [1]Institut für Strahlenphysik, Helmholtz-Zentrum Dresden - Rossendorf, Dresden, Germany — [2]Zentrum für Mikrotechnologien, Tech. Univ. Chemnitz, Chemnitz, Germany — [3]Institut für Physik, Univ. Halle, Halle, Germany — [4]Fraunhofer ENAS, Chemnitz, Germany

The first results on in-situ investigations of pore formation in ultra low-k dielectrics during a curing process, i.e., a porogen removal by vacuum annealing will be presented. The main focus is to obtain insight into initial stages of pore networks formation up to their full development. The in-situ annealing and Doppler broadening positron annihilation spectroscopy measurements have been conducted on our Apparatus for In-situ Defect Analysis (AIDA) - the end-station of a slow positrons beamline at HZDR. In addition, positron lifetime spectroscopy has been utilized, where mono-energetic pulsed positron beam (MePS) serves as a probe to evaluate pore sizes, their concentration and distribution as a function of curing temperature and time. The MePS facility has partly been funded by the Federal Ministry of Education and Research (BMBF) with the grant PosiAnalyse (05K2013). The AIDA system was funded by the Impulse- und Networking fund of the Helmholtz-Association (FKZ VH-VI-442 Memriox) and through the Helmholtz Energy Materials Characterization Platform (03ET7015).

KFM 24.6 Thu 11:40 E 124

Investigation of the porous structure of oblique angle deposited thin films with tailored architectures using Positron Annihilation Spectroscopy — •Maik Butterling[1], Agustín González-Elipe[2], Maciej Oskar Liedke[1], Aurelio García-Valenzuela[2], Rafael Alvarez Molina[2], Alberto Palmero Acebedo[2], Jorge Gil-Rostra[2], Victor Rico Gavira[2], Eric Hirschmann[1], Reinhard Krause-Rehberg[3], and Andreas Wagner[1] — [1]Institut für Strahlenphysik, Helmholtz- Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Laboratory of Nanotechnology on Surfaces, Instituto de Ciencia de Materiales de Sevilla (CSIC-Universidad de Sevilla), Seville, Spain — [3]Insitut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

Oblique angle deposited (OAD) thin films offer many possibilities for tailoring their microstructure for specific applications, which are typically linked with the high fraction of void space and porosity available in these thin films (typically of 50% or more from the total volume of the films) and the possibility of tailoring their microstructure in the form of slanted, chiral, zig-zag or similar nanostructures. For applications, control and precise knowledge of the porous structures is essential which can be studied by means of Positron Annihilation Spectroscopy. We will present the first results for the investigation of three different nano-columnar systems which have been studied using the slow-positron source MePS at HZDR. The MePS facility has partly been funded by the Federal Ministry of Education and Research (BMBF) with the grant PosiAnalyse (05K2013).

KFM 24.7 Thu 12:00 E 124

Bound state resonances as a simplified model for the scaling of Compton profiles — •Jakob Bonart, Michael Sekania, and Liviu Chioncel — TP III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Germany

We recently showed that the shape of the Compton profiles of crystalline alkali metals can be fitted by a q-Gaussian distribution [M. Sekania et al., Physica A 489C, 18-27 (2018)], which implies a novel type of scaling of the Compton profiles. Here we discuss the correspondence between Compton scattering and the process in which a non-relativistic bound state absorbs a momentum. In our simplified model we derive the transition probability into the nth-bound level, demonstrate its scaling through the q-Gaussian scaling function, and connect the q-parameter to the shape of the confining potential. We propose that this mechanism causes the scaling of the Compton profiles of alkali metals.

KFM 25: Ferroics and Multiferroics (joint session KFM/TT/MA)

Time: Thursday 9:30–13:30 Location: EMH 225

KFM 25.1 Thu 9:30 EMH 225

A piezoresponse force microscopy study of Bi(Fe,Sc)O3 multiferroic ceramics — •Vladimir Shvartsman[1], Andrei Salak[2], Dmitry Khalyavin[3], and Doru Lupascu[1] — [1]Institute for Material Science, University of Duisburg-Essen, Essen, Germany — [2]Department of Materials and Ceramic Engineering/CICECO, University of Aveiro, Aveiro, Portugal — [3]ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, UK

Bismuth ferrite (BFO) has attracted an immense attention as a rare room-temperature single-phase multiferroics. The magnetic and ferroelectric structure of BFO can be tuned by cationic substitutions. In particular, using the high-pressure synthesis method BiFe(1-x)Sc(x)O3 ceramics can be sintered. The material appears in different polymorphs. The phase obtained by quenching under pressure is antipolar, but can be irreversibly turned into a polar one by thermal cycling at normal pressure. The resulting modification is a rare example of coexistence of canted ferroelectric and ferromagnetic states. We have addressed ferroelectric properties of these materials by piezoresponse force microscopy (PFM). The post-annealed Bi(Fe0.5Sc0.5)O3 ceramics show a strong PFM signal and posses a well-developed domain pattern typical of a ferroelectric state. The quenched ceramics, however, demonstrate no piezoresponse that is in line with its antiferroelectric state. We found that this state can be transferred to a ferroelectric one by application of a strong enough electric field. The temporal and temperature stability of the induced states are studied.

KFM 25.2 Thu 9:50 EMH 225

Electronic Ferroelectricity in Organic Charge-Transfer Salts — •Jonas K. H. Fischer[1], Peter Lunkenheimer[1], Rudra Manna[2,3], Harald Schubert[3], Jens Müller[3], Michael Lang[3], Stephan Krohns[1], John A. Schlueter[4], Cecile Mézière[5], Patrick Batail[5], and Alois Loidl[1] — [1]Experimental Physics V, EKM, University of Augsburg, Augsburg, Germany — [2]Department of Physics, IIT Tirupati, Tirupati 517506, India — [3]Phys. Inst. Univ. Frankfurt, SFB/TR 49, Frankfurt, Germany — [4]Materials Research, National Science Foundation, Arlington, Virginia, United States — [5]Laboratoire MOLTECH, UMR 6200 CNRS-Université d'Angers, Bt. K, UFR Sciences, Angers, France

The often intriguing dielectric properties of the EDT-TTF-based charge-transfer salts have attracted considerable attention in recent years [1]. Examples are κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl, which exhibits multiferroicity [2], as well as α-(BEDT-TTF)$_2$I$_3$, which shows the signature of relaxor-ferroelectric behavior [1].
Here, we will present an overview of the dielectric properties of the above systems and provide new results on κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Cl, which also shows ferroelectric behavior in its charge-ordered state. In addition, further organic candidates for ferroelectricity as well as recent results on δ-(EDT-TTF-CONMe$_2$)$_2$Br are presented. The latter compound exhibits charge order but lacks dimerization. It displays interesting glasslike relaxation dynamics.
[1] P. Lunkenheimer and A. Loidl, J. Phys.: Condens. Matter **27**, 373001 (2015). [2] P. Lunkenheimer *et al.*, Nat. Mater. **11**, 755 (2012).

KFM 25.3 Thu 10:10 EMH 225

Superconductivity and ferroelectric quantum criticality in KTaO3 — •Tobias Esswein, Awadhesh Narayan, and Nicola Spaldin — Materials Theory, ETH Zurich, Wolfgang-Pauli-Strasse 27, CH-8093 Zurich, Switzerland

Electron doped cubic perovskite KTaO3 has recently been shown to become superconducting [1]. In the closely related material SrTiO3, a ferroelectric quantum critical point was proposed to be the origin of superconductivity [2]. In this work, using first-principles calculations, we show that a ferroelectric quantum critical point emerges with electron doping in KTaO3, lying at doping values close to the top of the superconducting dome. We examine the effects of larger spin-orbit coupling and absence of crystal field splitting in KTaO3, in comparison to SrTiO3, on the phonon spectrum, electron-phonon coupling and quantum oscillations. Our findings contribute to the growing understanding of superconductivity around quantum critical points and could help in designing materials with higher superconducting critical temperatures.

[1] Ueno, K. et al. Discovery of Superconductivity in KTaO3 by

Electrostatic Carrier Doping. Nature Nanotechnology 6, 408 (2011). [2] Edge, J. M., Kedem, Y., Aschauer, U., Spaldin, N. A. & Balatsky, A. V. Quantum Critical Origin of the Superconducting Dome in SrTiO3. Physical Review Letters 115, 247002 (2015).

KFM 25.4 Thu 10:30 EMH 225

In-operando study of polarization reversal in ferroelectric thin films — •Christelle Kwamen[1], Matthias Rössle[2], Matthias Reinhardt[1], Wolfram Leitenberger[2], Flavio Zamponi[2], Marin Alexe[3], and Matias Bargheer[1,2] — [1]Helmholtz Zentrum Berlin — [2]Institute of physics and astronomie, University of Potsdam — [3]Department of physics, University of Warwick

The mechanisms associated with polarization reversal in ferroelectric materails are still under investigations because the microscopic dynamics are not yet fully understood. The permanent quest for energy efficient technologies drives investigations on making a ferroelectric operational under lowest switching voltage. There are many studies which investigate either the electrical signature of the switching or the structural changes of the crystal lattice associated with the switching. We present here a simultaneous study of the electrical and structural responses of a lead-zirconate-titanate-based capacitor heterostructure during charging, discharging, and polarization reversal, using time-resolved X-ray diffraction. Concomitant with the ferroelectric current peak, we observe the switching is characterized by a transient disorder evidenced by a decrease of the Bragg peak intensity. A peak width increase reveals the domain dynamics during the reversal. Our investigations show how the incomplete screening of the depolarization charges affect the piezoelectric response, measured via the Bragg peak position. We examine the interplay between charge flow, atomic motion in real time during device operation. We investigate how ultrashort laser pulse excitation can increase the charge flow in a biased device.

KFM 25.5 Thu 10:50 EMH 225

Domains Properties in Thin Ferroelectric Films Related to Surface Screening, Flexoelectric and Vegard Effects — •Ivan S. Vorotiahin[1,2], Anna N. Morozovska[2], Eugene A. Eliseev[3], Sergei V. Kalinin[4], Qian Li[4], Yevhen M. Fomichov[3,5], and Yuri A. Genenko[1] — [1]Institut für Materialwissenschaft, Technische Universität Darmstadt, Darmstadt, Germany — [2]Institute of Physics, National Academy of Sciences of Ukraine, Kyiv, Ukraine — [3]Institute for Problems of Materials Science, National Academy of Sciences of Ukraine, Kyiv, Ukraine — [4]The Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, USA — [5]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

Ferroelectric domains is a topic of undying interest in the research community, since their properties and formation conditions still remain not fully understood. Among those conditions, surface screening charges, flexoelectric effect and chemical stresses can be named. Their influence is well observable in films of several to several tens of nanometres thicknesses, i.e. in the forefront of the phenomenological theories.

A series of modelling experiments has been performed to predict the effects that those physical qualities can make on a shape of ferroelectric domains in the most well-known perovskite materials, as well as their impact on the electromechanical properties, phase diagrams, and field distributions. Their influence has been numerically and analytically estimated to provide a roadmap for future measurements and compared with each other to obtain a stronger understanding of the physical processes occurring in perovskites.

KFM 25.6 Thu 11:10 EMH 225

Screening in metallized ferroelectrics — •Hongjian Zhao[1], Alessio Filippetti[2,3], Carlos Escorihuela-Sayalero[1], Pietro Delugas[4], Enric Canadell[5], Laurent Bellaiche[6], Vincenzo Fiorentini[2,3], and Jorge Íñiguez[1] — [1]Materials Research and Technology Department, Luxembourg Institute of Science and Technology, Luxembourg — [2]Dipartimento di Fisica, Università di Cagliari, Cittadella Universitaria, Italy — [3]CNR-IOM SLACS, Cittadella Universitaria, Italy — [4]Scuola Internazionale Superiore di Studi Avanzati, Italy — [5]Institut de Ciència de Materials de Barcelona, Spain — [6]Physics Department and Institute for Nanoscience and Engineering, University of Arkansas, USA

Ferroelectric materials are characterized by spontaneous polar distortions. The behavior of such distortions in the presence of free charge is the key to the physics of metallized ferroelectrics in particular, and of structurally-polar metals more generally. Using first-principles simulations, here we show that polar distortions resist metallization and the attendant suppression of long-range dipolar interactions in the vast majority of a sample of eleven representative ferroelectrics. We identify a novel meta-screening effect, occurring in the doped compounds as a consequence of the charge rearrangements associated to electrostatic screening, as the main factor determining the survival of a non-centrosymmetric phase. Our findings advance greatly our understanding of the essentials of structurally-polar metals, and offer guidelines on the behavior of ferroelectrics upon field-effect charge injection or proximity to conductive device elements.

20 min. break

KFM 25.7 Thu 11:50 EMH 225

Pressure-induced insulator-metal transition in $EuMnO_3$ — •Andres Cano — CNRS, Univ. Bordeaux, ICMCB, Bordeaux, France

We study the influence of external pressure on the electronic and magnetic structure of $EuMnO_3$ from first-principles calculations. We find a pressure-induced insulator? metal transition at which the magnetic order changes from *A*-type antiferromagnetic to ferromagnetic with a strong interplay with Jahn?Teller distortions. This unexpected pressure-induced insulator-to-metal transition, although similar to the observed in CMR $LaMnO_3$, is unprecedented within the multiferroic $RMnO_3$ series. In addition, we find that the non-centrosymmetric $E^?$-type antiferromagnetic order can become nearly degenerate with the ferromagnetic ground state in the high-pressure metallic state. These features make $EuMnO_3$ an unique compound among the manganites because it behaves differently with respect to physical and "chemical" pressure, and hosts a genuinely new type of ferroelectric-like metallic state.

[1] *Pressure-induced insulator-metal transition in EuMnO3*, R. Qiu, E. Bousquet and A. Cano, J. Phys.: Condens. Matter 29, 305801 (2017).

KFM 25.8 Thu 12:10 EMH 225

Far infrared studies on a diluted rare-earth langasite — •Lorenz Bergen[1], Evan Constable[1], Lukas Weymann[1], Alexander A. Mukhin[2], Nadezhda Kostyuchenko[1], and Andrei Pimenov[1] — [1]Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Prokhorov General Physics Institute, Russian Academy of Sciences, 119991 Moscow, Russia

Rare-earth langasites demonstrate fascinating structural and magnetic effects such as geometric frustration and are possible candidates for the spin-liquid state. To better understand the interplay between the structural and magnetic properties it is important to study the phonon and crystal electric field spectra that can be observed in the far infrared (FIR) range. The langasite structure crystallizes in the P321 space group with a general formula $A_3BC_3D_2O_{14}$. Here we present spectra of the diluted rare-earth langasite $La_{2.91}Ho_{0.09}Ga_5SiO_{14}$ using polarized far infrared radiation along different crystallographic directions and under a broad temperature range. The observed phonon frequencies are compared with model calculations. We compare the results on the holmium doped crystal and on pure $La_3Ga_5SiO_{14}$ langasite.

KFM 25.9 Thu 12:30 EMH 225

Magnetic Excitations and High-Order Magnetoelectric Effect in Holmium Langasite — •Lukas Weymann[1], Thomas Kain[1], Alexey Shuvaev[1], Artem Kuzmenko[2], Alexander Mukhin[2], Evan Constable[1], Lorenz Bergen[1], Nadezhda Kostyuchenko[1], Anna Pimenov[1], and Andrei Pimenov[1] — [1]Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Prokhorov General Physics Institute, Russian Academy of Sciences, 119991 Moscow, Russia

Recently, compounds of the langasite family (prototype $La_3Ga_5SiO_{14}$) have attracted considerable attention due to their intriguing magnetic and magnetoelectric properties. The geometric frustration of the magnetic ions lies in the focus of the investigation of rare-earth langasites, since this makes them promising candidates for spin liquids.

In this work we show that in diluted rare-earth langasite $La_{2.91}Ho_{0.09}Ga_5SiO_{14}$ (3%Ho-LGS), where no magnetic frustration is present, unusual properties can be observed. 3%Ho-LGS single crystals reveal a substantial magnetoelectric effect comparable with other rare-earth langasites. The symmetry and the field dependence of the effect can only be explained by taking into account the higher order expansions of the crystal field theory. Terahertz measurements with a

Mach-Zehnder interferometer reveal a series of characteristic magnetic excitations and a strong zero-field mode of presently unknown origin.

KFM 25.10 Thu 12:50 EMH 225

Structural phase transition and domain formation in the hybrid improper ferroelectric $Ca_3Mn_{1.9}Ti_{0.1}O_7$ — •Mads C. Weber[1], Thomas Lottermoser[1], Morgan Trassin[1], Bin Gao[2], Sang-Wook Cheong[2], and Manfred Fiebig[1] — [1]ETH Zurich, Switzerland — [2]Rutgers University, Piscataway, New Jersey, USA

One of the bottlenecks for the application of magneto-electric multiferroics is the lack of materials with both, a robust coupling between ferroelectricity and magnetism, and a sufficiently large polarization. This problem may be overcome in layered perovskite systems, where octahedral rotations can give rise to improper ferroelectricity as well as a net-magnetization. Accordingly, ferroelectricity and magnetic order are linked by non-polar structural distortions. Essential for the understanding of the potential coupling of both parameters is an in-depth comprehension of the structural distortions and the formation of domains. In this work, we present a combined Raman spectroscopy (RS) and optical second harmonic generation (SHG) study of the improper ferroelectric phase transition and the related domain formation. Using RS, we trace the evolution of the non-polar structural distortions across the phase transition by probing the lattice vibrations of the system. Furthermore, we investigate the emergence of ferroelectricity by SHG a technique highly sensitive to breaking of inversion symmetry. Hence, RS and SHG represent a unique combination to investigate improper ferroelectric phase transitions.

KFM 25.11 Thu 13:10 EMH 225

Lead Palladium Titanate: A new room-temperature magnetoelectric multiferroic — •Elzbieta Gradauskaite[1,2], Jonathan Gardner[3], Rebecca M. Smith[3], Finlay D. Morrison[3], Stephen L. Lee[1], Ram S. Katiyar[4], and James F. Scott[1,3] — [1]School of Physics and Astronomy, University of St Andrews, United Kingdom — [2]Present address: Department of Materials, ETH Zürich, Zürich, Switzerland — [3]School of Chemistry, University of St Andrews, United Kingdom — [4]Department of Physics, SPECLAB, University of Puerto Rico, USA

Magnetoelectric multiferroic materials combine the advantages of FeRAMs (speed, low power) and MRAMs (non-destructive readout) due to the linear (magnetoelectric) coupling between ferroelectricity and ferromagnetism. Despite the worldwide interest and effort, very few single-phase materials have been discovered that exhibit magnetoelectric coupling at room temperature. Until very recently $BiFeO_3$ was the only one, however it is not suitable for real practical device applications due to high leakage currents and weak coupling. Here, we demonstrate that $PbTi_{1-x}Pd_xO_3$ ($0 < x < 0.3$) is multiferroic up to 400 K and possesses a strong magnetoelectric coupling. This observation is remarkable because Pd is difficult to substitute into ABO_3 perovskite oxides and it is magnetic only under unusual conditions (strain or internal electric fields). Dielectric spectroscopy and magnetization studies will be discussed in detail, while paying particular attention to secondary phases present in the bulk specimen, identified as PdO, $PbPdO_2$ and Pd_3Pb using PXRD, SEM, EDX and XPS.

KFM 26: Lithography IV: Lithography and Structuring (joint session KFM/DS)

This second lithography session focuses mainly on the application of advanced methods for quantum applications and the fabrication of lower dimensional systems. With the mass production of transistors devices at the 10 nm level with transmissive optical masks and with extreme UV reflective masks being at the horizon for mass fabrication, the industrial photomask fabrication is currently facing a significant technology transition and new technology requirements needed to keep pace with. The session also looks into those industrial challenges. Finally, the session focuses on important characterization methods required for the above mentioned state-of-the art lithography methods and their characterization.

Organizer: Robert Kirchner - Technische Universität Dresden

Time: Thursday 15:00–18:10 Location: EMH 025

Invited Talk KFM 26.1 Thu 15:00 EMH 025

Electron Beam Lithography and Ion Beam Patterning for Applications in Quantum Technology — •Jörg Stodolka, Michael Kahl, Axel Rudzinski, and Sven Bauerdick — Raith GmbH, Dortmund, Germany

Electron Beam Lithography and Ion Beam Patterning allow to fabricate structures with nm resolution and accuracy, which is required for many devices based on quantum technology. After a general overview we present two specific applications.

First, we show an approach for a deterministic realization of photonic devices with very high process yield utilizing cathodoluminescence spectroscopy (CL) in combination with electron beam lithography: An electron beam is used to write nanopatterns in resist at positions that are preselected by local generation of light detected by CL.

Second, we present a method for scalable and maskless fabrication of silicon vacancy (VSi) defect arrays in silicon carbide using focused ion beam. The photoluminescence spectrum and optically detected magnetic resonance of the generated defect spin ensemble are used to analyze the synthesized centers and their desired defect state. The reliable production of VSi defects with a dedicated focused ion beam system allowing single ion implantation could pave the way for applications in quantum photonics and quantum information processing.

KFM 26.2 Thu 15:30 EMH 025

Technology for fabrication of suspended sub-5 nm silicon nanowires and applications thereafter — Nikolay Petkov[1] and •Yordan M. Georgiev[2] — [1]Tyndall National Institute, University College Cork, Lee Maltings, Dyke Parade, Cork, T12R5CP, Ireland — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Bautzner Landstrasse 400, 01328 Dresden, Germany

Si nanowires (Si NWs) are very promising as channels for field effect transistors (FETs) and also as sensing devices. When the NW diameter is in the sub-10 nm range, quantum confinement of carriers is observed at room temperature, which is very appealing from scientific and application point of view.

This paper will present a technology for fabrication of sub-5 nm suspended Si NWs on silicon-on-insulator wafers. News of 20 nm width are first defined in the top Si layer by electron beam lithography and reactive ion etching. Then the NWs are subjected to three consecutive cycles of rapid thermal oxidation in oxygen atmosphere and wet etching in hydrofluoric acid. The resulting suspended Si NWs have high-quality crystalline structure and sub-5 nm size.

The possible applications of such NWs will be discussed, including FET-based Si NW chemo-/biosensors as well as gate all around (GAA) FETs. Additionally, the development of self-aligned nickel silicide NW contacts will be presented. The formation mechanism was examined by in-situ electron microscopy as a function of NW diameter and surface oxide.

KFM 26.3 Thu 15:50 EMH 025

Photomask Manufacturing Technology - An Overview — •Christian Buergel, Torben Heins, and Martin Sczyrba — AMTC Dresden, Raehnitzer Allee, 0199 Dresden, Germany

Semiconductor devices are designed as vertical stacks of electrical components (e.g. transistors, capacities, wiring and connections), which are manufactured layer by layer during wafer processing.

Pattern formation on the wafer is done by using projection lithography and photomasks are key elements for the lithography. At least one photomask is required for each layer, where the mask contains the design information and is used as master for the desired geometries. The design, as represented on the photomasks, is replicated as a 4x demagnified image onto the wafer in the desired amount, hence enabling

rapid and cost effective semiconductor production.

This presentation will give a broad overview of the manufacturing chain of a photomask. It will introduce into required processes like data preparation and manipulation for mask writing, resist and absorber material processing, metrology and inspection as well as mask repair and its qualification.

KFM 26.4 Thu 16:10 EMH 025

Simulation of Ion Beam induced Surface Dynamics — •Alrik Stegmaier and Hans Hofsäss — 2. Physikalisches Institut, Georg-August Universität Goettingen

Structuring of surfaces through ion beam irradiation can be used to create self organizing dune-like waves, dimples, flat surfaces or chaotic patterns. The final structures are a result of the interplay of sputtering, redeposition, projectile implantation, transport and viscous flow, void/bubble formation and the initial surface conditions.

Accurate simulations of structuring are possible through molecular dynamics simulations, but these simulations are computationally too expensive to allow for a prediction of up to micrometer scale structure. A much faster approach is available through the use of continuum models. For this the net effect of the irradiation is expressed as the local change in surface height as a function of and up to forth order spacial derivatives of the local surface height. Typically the resulting equations of motion are taylor-expanded up to second order. Such an approach can be accurate when the surface is relatively flat and shadowing is not important, but the parameters often need to be empirically readjusted for experiments at different impact angles, ion energies or materials.

Here we present a new software package that allows for the rapid simulation of surface dynamics for arbitrary, nonlinear equations of motion that can also include nonlocal effects. With this software we explore nonlinear expansions to some of the common models, the effects of shadowing at flat impact angles and parameter determination through binary collision approximation simulation.

20 min. break

KFM 26.5 Thu 16:50 EMH 025

NFFA-Europe: enhancing European competitiveness in nanoscience research and innovation — •Dimitrios Kazazis — Paul Scherrer Institut, 5232 Villigen, Switzerland

NFFA-Europe is a European open-access resource for experimental and theoretical nanoscience. It brings together advanced infrastructures throughout Europe, specialized on growth, nanolithography, nanocharacterization, theory, simulation and fine-analysis with Synchrotron, FEL and Neutron radiation sources to create a multi-site research platform that enables European and international researchers to carry out advanced project proposals impacting science and innovation. NFFA-Europe coordinates access to infrastructures on different aspects of nanoscience research that are not currently available at single specialized sites. Technique and tool selection, proposal construction and submission are all done through a single and intuitive web portal. The access to the combined infrastructures through NFFA-Europe is centrally coordinated and free of charge for all technologically feasible and internationally peer-reviewed and approved user projects. Not only do the approved projects have access to the combined infrastructures, but they also benefit from the competences and the technical support of the NFFA sites as well as a contribution towards travel and subsistence costs. NFFA-Europe's internal joint research activities address key bottlenecks of nanoscience and nanotechnology i.e. nonostracture traceability, protocol reproducibility, in-operando nanomanipulation and analysis, open data etc. (www.nffa.edu)

KFM 26.6 Thu 17:10 EMH 025

Fresnel-Mirror-Setup for Interference Lithography — •Arrigo Facchini[1], Bodo Fuhrmann[2], Hartmut S. Leipner[2], Georg Schmidt[1,2], and Roland Scheer[1] — [1]Martin Luther University Halle-Wittenberg Institute of Physics, D-06099 Halle (Saale), Germany — [2]Martin Luther University Halle-Wittenberg Interdisciplinary Center of Materials Sciences, D-06099 Halle (Saale), Germany

Interference lithography is one of many alternative lithography techniques for the fast fabrication of large area regular nano- and microscale patterns. A variety of more or less complex setups using Lloyd*s interferometers or beam splitters are described in literature.

In particular, rigid Lloyd*s interferometer setups allow the fast change of the periodicity by simply changing the angle of incidence. They have, however, the drawback that for smaller angles of incidence (larger periodicity) the illuminated area decreases and as a consequence also the possible sample size.

Here a robust Fresnel mirror setup is presented, which overcomes this problem and allows the fast fabrication of regular patterns in the *m-range with freely selectable periodicity. The maximum sample size is only determined by the setup chosen.

KFM 26.7 Thu 17:30 EMH 025

Analysis of rough nanostructured surfaces by EUV-scatterometry — •Analía Fernández Herrero, Frank Scholze, and Victor Soltwisch — Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin, Germany

Lamellar-gratings are commonly-used as diffractive optical elements or in state-of-the-art integrated electronic circuits. For the control of the lithographic manufacturing process in semiconductor manufacturing a rapid in-line characterization of the nanostructures is indispensable. With shrinking structure sizes, roughness gains influence on the device performance. Therefore the analysis of nanostructured surfaces demands the development of new metrology tools capable of destruction-free measurements, which, at the same time, deliver statistical information, relevant for the study of the imperfections. Small angle X-ray scattering under grazing incidence has already been investigated for the determination of the geometry parameters of such structures. Several reports stress the importance of the identification of the roughness contributions. Using EUV or soft X-ray radiation, with longer wavelengths, larger incidence angles can be used reducing the beam footprint on the samples without compromising the surface sensitivity. We present a new experimental tool to be developed at the PTB soft X-ray beamline at the electron storage ring BESSY II for the measurement of small structures and roughness contributions based on soft X-ray and EUV scatterometry.

KFM 26.8 Thu 17:50 EMH 025

GISAXS reconstruction of profiles of gratings produced by quadruple patterning — •Mika Pflüger[1], Victor Soltwisch[1], R. Joseph Kline[2], Frank Scholze[1], and Michael Krumrey[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), Berlin, Germany — [2]National Institute of Standards and Technology (NIST), Gaithersburg, United States

New approaches are needed for the fast, non-destructive dimensional measurement of complex nanostructures produced in the semiconductor industry. One technique being considered is Small-Angle X-ray Scattering (SAXS), which has already been used to reconstruct the line profile of gratings with low uncertainties. Grazing-Incidence SAXS (GISAXS) additionally provides surface sensitivity, but the interpretation of the scattering is complicated by multiple scattering effects.

To produce structures beyond the diffraction limit of a single lithographic exposure, self-aligned double patterning (SADP) can be used. In SADP, sidewalls are deposited on the original line and the original line is removed, such that the sidewalls form lines with a doubled structure density. If the sidewall width and the original linewidth do not match, an alternating pitch error is introduced, impacting the performance of the resulting structures.

We present GISAXS measurements of a sample series produced by self-aligned quadruple patterning with varying pitch errors. From the intensities of the grating diffraction orders, we quantify the pitch errors and compare our results to previous SAXS measurements of the same samples.

KFM 27: Postersession KFM

Time: Thursday 15:00–17:00 Location: Poster E

KFM 27.1 Thu 15:00 Poster E

Frequency shifts and Raman signatures at ferroelectric domain interfaces of $LiNbO_3$ and $LiTaO_3$ — Sergej Neufeld[1], Michael Rüsing[1], •Simone Sanna[2], Gerhard Berth[1], Artur Zrenner[1], and Wolf Gero Schmidt[1] — [1]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [2]Justus-Liebig-Universität Giessen, Institut für Theoretische Physik, 35392 Gießen, Germany

Periodically poled lithium niobate ($LiNbO_3$, LN) and lithium tantalate ($LiTaO_3$, LT) structures are of particular technological interest as waveguides and SHG structures. The interface between neighboring domains features a large polarization gradient, which is accompanied by a modulation of numerous physical properties such as internal strain, birefringence and Raman cross section. In recent years, several experimental techniques, including Raman spectroscopy [1], have been utilized to image domain walls. In this work, vibrational properties and Raman signatures of LN and LT in the vicinity of domain walls are studied phenomenologically within an atomistic model via density functional theory calculations. Additionally, Raman signatures of LN and LT domain walls are studied experimentally via a confocal Raman setup. The frequency shifts and Raman intensities of E and A_1 modes calculated along a phenomenological reaction coordinate between both phases are in qualitative agreement with the measured data. In particular, the well-known soft mode behavior of the low frequency A_1-TO_1 mode is reproduced in the calculations.

[1] Appl. Phys. B 78, 363-366 (2004)

KFM 27.2 Thu 15:00 Poster E

Ferroelastic domain identification in $BiFeO_3$ crystals using Raman spectroscopy — •Jan Rix[1], Cameliu Himcinschi[1], Christian Röder[1], Martin Rudolph[2], Mingmin Yang[3], David Rafaja[2], Jens Kortus[1], and Marin Alexe[3] — [1]Institute of Theoretical Physics, TU Bergakademie Freiberg, 09596 Freiberg, Germany — [2]Institute of Materials Science, TU Bergakademie Freiberg, 09596 Freiberg, Germany — [3]Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom

Multiferroic $BiFeO_3$ crystals have been investigated by means of Raman spectroscopy using 442 nm (resonant conditions) and 633 nm (non-resonant conditions) laser wavelengths. The azimuthal angular dependence of the intensity of the Raman modes allowed an assignment to one of five symmetry characters, which are present in the directional dispersion [1,2]. Mixed symmetries were taken in account, considering the orientation of the optical c-axis along the pseudo-cubic $<111>_{pc}$ direction. The experimental data have been verified by a Raman tensor formalism simulation. The strong intensity variation of the polar Raman modes at 138 cm^{-1} ($\mathbf{E}_{TO}$ - $\mathbf{A}_{1TO}$) and at 172 cm^{-1} ($\mathbf{A}_{1LO}$ - $\mathbf{E}_{LO}$) were used for line scans, mappings and a depth profile in order to identify the elastic domain patterns. The distribution of domains found by Raman spectroscopy is in very good agreement with the domain pattern revealed by Electron Back Scattering Diffraction (EBSD) and Piezo-Force Microscopy (PFM).

[1] J. Hlinka et al. Phys. Rev. B 83, 020101 (2011). [2] A. Talkenberger et al. J. Raman Spectrosc. 46, 1245 (2015).

KFM 27.3 Thu 15:00 Poster E

Domain evolution in a Ba(Zr0.2Ti0.8)O3-0.5(Ba0.7Ca0.3)TiO3 piezoceramic studied by piezoresponse force microscopy — •Xijie Jiang, Na Liu, Robert Stark, and Christian Dietz — Technische Universität Darmstadt, Alarich-Weiss-Str. 16, Darmstadt, Germany

Lead-free (1-x)Ba(Zr0.2Ti0.8)O3-x(Ba0.7Ca0.3)TiO3 (BZT- xBCT) ceramics have drawn special attention to researchers because of their outstanding dielectric and electromechanical properties, competitive to lead zirconate titanate (PZT). In particular, BZT-0.5BCT was reported to have a piezoelectric coefficient of 620 pC/N explained by the existence of a triple point close to room temperature. However, the fundamental mechanisms behind the functionality of this ferroelectric are not completely understood. Here, we use piezoresponse force microscopy (PFM) to observe the domain evolution of a BZT-0.5BCT ceramic while changing the temperature and the applied voltage between tip and sample. In the initial state, the sample exhibits a combination of wedge-shaped and lamellar domains. During the increase of the applied voltage to +30 V, the observed area formed a single domain state. Subsequently decreasing the applied voltage step-wise to -30 V and increasing back to 0 V caused the sample to form wedge-shaped and lamellar domain again. Thus, the sample reversibly transforms from a multi-domain to a single-domain state during a complete poling cycle. During heating to 60 °C, most wedge-shaped domains transformed to lamellar domains and the orientation of the domain configuration was partially reversed.

KFM 27.4 Thu 15:00 Poster E

Towards a proof of water splitting via pyroelectrolysis — •Thomas Köhler, Wolfram Münchgesang, Erik Mehner, Juliane Hanzig, Hartmut Stöcker, and Dirk C. Meyer — Institut für Experimentelle Physik, Technische Universität Bergakademie Freiberg, Leipziger Str. 23, 09599 Freiberg, Germany

The generation of hydrogen through water electrolysis has been understood for a long time and will be used for large-scale conversion of electrical energy into chemical energy in the future. The direct conversion of residual heat into hydrogen is completely new to our knowledge, but feasible when making use of pyroelectric materials. In pyroelectrolysis, a cyclic temperature excitation generates an electric field between the crystal surfaces due to an imbalance between polarization and compensation charges. For water electrolysis, this electric field must exceed the redox potential of water.

A pyroelectolysis cell was developed for investigating the interaction of congruent $LiTaO_3$ with aqueous media, in order to record the surface potential during the temperature change and the reaction rate of the pyroelectolysis. A sufficiently high voltage difference between the opposite crystal surfaces caused by cyclic temperature changes was observed. This satisfies the basic requirement for water splitting on the pyroelectric surface. Cyclic voltammetry of the electrolyte solution was applied for electrochemical detection of the water splitting reaction. To finally prove water splitting, the increasing educt concentration in the electrolyte solution would be monitored as a change of the oxidation and reduction peaks.

KFM 27.5 Thu 15:00 Poster E

Anisotropic Transport of the 2D Electron System in (001) Al_2O_{3-d}/SrTiO3 Heterostructures — •Karsten Wolff[1], Roland Schäfer[1], Richard Thelen[2], Matthias Meffert[3], Dagmar Gerthsen[3], Rudolf Schneider[1], and Dirk Fuchs[1] — [1]Karlsruher Institut für Technology, Institut für Festkörperphysik — [2]Karlsruher Institut für Technology, Institut für Mikrostrukturtechnik — [3]Karlsruher Institut für Technology, Laboratorium für Elektronenmikroskopie

Transport measurements on the two-dimensional electron system in $Al_2O_3/SrTiO_3$ heterostructures indicate significant non-crystalline anisotropic behavior below T ≈ 30 K. Lattice dislocations in $SrTiO_3$ and interfacial steps are suggested to be the main sources for electronic anisotropy in (001) oriented heterostructures. Anisotropic defect scattering likewise alters magnetoresistance at low temperature remarkably and influences spin-orbit coupling significantly by the Elliot-Yafet mechanism of spin relaxation resulting in anisotropic weak localization. Applying a magnetic field parallel to the interface results in an additional field-induced anisotropy of the magnetoconductance, which can be attributed to Rashba spin-orbit interaction.

KFM 27.6 Thu 15:00 Poster E

Investigation of magneto-ionic effects on Au-Fe (core-shell) nanowires — •Martin Nichterwitz[1,2], Shashank Honnali[1], Tom Sieger[1], Diana Pohl[1], Anna Niemann[1], Kornelius Nielsch[1], and Karin Leistner[1] — [1]IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — [2]Technische Universität Dresden, Physikalische Chemie, 01062 Dresden, Germany

Miniaturization and the demand for low-power devices led to increasing research of voltage-controlled devices, which do not show effects like joule heating. It was recently shown that reversible magneto-ionic manipulation with up to 64 % change in magnetization of Fe/FeOx films is possible at room temperature in liquid alkaline electrolytes. [1,2] The change of geometry from thin films to nanowires (NW) promises enhanced magneto-ionic effects due to the higher surface/volume ratio. We present an approach to observe the above stated effect using Au-

Fe-NWs (core-shell). Au-NWs are grown by electrodeposition into a nano-porous Al2O3-template. Individual Au-NWs are electrically contacted on a glass substrate using laser lithography and a metallization process. Subsequently, a 5-10 nm thick Fe shell is electrodeposited on the Au-NW. To investigate the magneto-ionic effects, in-situ measurements (resistivity and magnetization) will be performed under different potentials in liquid alkaline electrolytes. This is expected to lead to the reversible switching between ferromagnetic and non-ferromagnetic states in the Fe/FeOx shell on the NW, due to reduction and oxidation processes, respectively. [1] K. Duschek et al., Electrochem. Comm. 72, 2016, 153 [2] K. Duschek et al., APL Mater. 4, 2016, 032301

KFM 27.7 Thu 15:00 Poster E

Interplay of oxygen vacancies and conductance in SrMnO3 thin films under epitaxial tensile strain — Lokamani Lokamani[1], Carina Faber[3], Peter Zahn[1], Nicola Spaldin[3], and •Sibylle Gemming[1,2] — [1]Institute of Ion Beam Physics and Materials Research, HZDR, 01314 Dresden, Germany — [2]Institute of Physics, Technische Universität, 09107 Chemnitz, Germany — [3]Materials Theory, ETH, 8093 Zürich, Switzerland

Strontium manganate (SrMnO3), a perovskite polymorph, exhibits cubic structure at low temperatures, which transforms under tensile strain into a G-type-antiferromagnetic (G-AFM) antiferrodistortive polar phase in the plane parallel to the substrate[1]. Recently, ferroelectric domains have been observed experimentally in 20nm thin films of SrMnO3 under 1.7% tensile strain on (001)-oriented LSAT grown in an oxygen-deficient atmosphere[2]. Strikingly, the individual domains show different conductance features, whereas the domain walls were found to be electrically insulating, rendering the domains to form stable nano-capacitors with high charge rention times.

Here, we present a detailed first-principle investigation of the domain wall formation in strained SrMnO3, their electronic properties and the influence of oxygen vacancies on the 2D-electron gas at the polar domain walls. Preliminary results on the migration energetics of the oxygen vacancies are expected.

[1] J. H. Lee et al., PRL 104, 207204 (2010)
[2] C. Becher et al., Nature Nanotechnology 10, 661 (2015)
Funding by VI Memriox(VH-VI-422) & Nanonet(VH-KO-606)

KFM 27.8 Thu 15:00 Poster E

Direct measurements of electrocaloric effect in Barium Titanate single crystals — •Maksim O. Karabasov, Mehmet Sanlialp, Vladimir V. Shvartsman, and Doru C. Lupascu — Institute for Materials Science, University of Duisburg-Essen, 45141 Essen, Germany

The electrocaloric effect (ECE) is studied for barium titanate single crystals utilizing two direct measurement methods. The adiabatic electrocaloric temperature change is observed by applying an electric field to the barium titanate single crystals in a quasi-adiabatic calorimeter. The second method uses the enthalpy change in a modified differential scanning calorimeter (DSC) to calculate the electrocaloric temperature change [1]. The focus of this study is to examine the anisotropy of ECE by applying electric fields for [001], [011] and [111] oriented single crystals. The anisotropy of the ECE leads to a possible negative temperature change, i.e. a temperature decrease by application of an electric field during the orthorhombic-tetragonal phase transition of Barium Titanate, if the field orientation favors the higher temperature/entropy phase [2].

[1] M. Sanlialp et al., Appl. Phys. Lett. **111**, 173903 (2017)
[2] M. Marathe et al., Phys. Rev. B **96**, 014102 (2017)

KFM 27.9 Thu 15:00 Poster E

Polaron optical absorption in congruent lithium niobate from time-dependent density-functional theory — •Michael Friedrich[1], W. G. Schmidt[1], Arno Schindlmayr[1], and Simone Sanna[2] — [1]Department Physik, Universität Paderborn, 33095 Paderborn, Germany — [2]Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen

The optical properties of congruent lithium niobate are analyzed from first principles. The dielectric function of the material is calculated within time-dependent density-functional theory. The effects of isolated intrinsic defects and defect pairs, including the Nb_{Li}^{4+} antisite and the Nb_{Li}^{4+}–Nb_{Nb}^{4+} pair, commonly addressed as bound polaron and bipolaron, respectively, are discussed in detail. In addition, we present further possible realizations of polaronic and bipolaronic systems. The absorption feature around 1.64 eV, ascribed to small bound polarons [1], is nicely reproduced within these models. Among the investigated defects, we find that the presence of bipolarons at bound interstitial-vacancy pairs Nb_V–V_{Li} can best explain the experimentally observed broad absorption band at 2.5 eV. Our results provide a microscopic model for the observed optical spectra and suggest that, besides Nb_{Li} antisites and Nb and Li vacancies, Nb interstitials are also formed in congruent lithium-niobate samples [2].

[1] O. F. Schirmer *et al.*, J. Phys.: Condens. Matter **21**, 123201 (2009).
[2] M. Friedrich *et al.*, Phys. Rev. Materials **1**, 054406 (2017).

KFM 27.10 Thu 15:00 Poster E

Broadband transient absorption spectroscopy of reduced lithium niobate after pulse excitation — •Stefan Hagedorn, Simon Messerschmidt, and Mirco Imlau — Department of Physics, Osnabrück University, Barbarastr. 7, 49076 Osnabrück, Germany

It is well known that transient absorption in lithium niobate (LN) can be studied by the use of single line pump and probe laser pulses [Imlau, M. *et al.*, Appl. Phys. Rev. 2 (2015)]. However, this technique inhibits access to the specific broadband absorption features of the underlying polaron species.

We have addressed this problem by installing a transient absorption spectrometer with a ns pulse laser as excitation source and a ns supercontinuum pulse laser ($\lambda = (400 - 1600)$ nm) as a probing source. Our setup is able to obtain temporal dynamics in the orders $(10^{-7} - 10^{3})$ s using an electronic delay between pump and probe pulses. For the first time we are able to show that the induced change of absorption in thermally reduced LN exhibit a transparency in the blue spectral region due to the depleted bipolarons and a significant absorption in the near-infrared induced by bound polarons. However, absorption maxima and minima are shifted from their denominated wavelengths compared to state of the art-knowledge. Using this setup, it is now possible to experimentally determine spectro-temporal absorption characteristics, e.g., to resolve polaron energy shifts caused by different pump wavelengths. This way, new insights to polaron dynamics beyond simplistic model extrapolations can be accessed. Financial support by the DFG (IM 37/5-2, INST 190/165-1 FUGG) is gratefully acknowledged.

KFM 27.11 Thu 15:00 Poster E

Dynamics of small polarons in the limit of high charge carrier densities — •Thorben Groven, Simon Messerschmidt, and Mirco Imlau — Department of Physics, Osnabrück University, Barbarastr. 7, 49076 Osnabrück, Germany

Small strong-coupling polarons take a crucial part in optical processes [Imlau, M. *et al.*, Appl. Phys. Rev. 2 (2015)]; therefore, polaron dynamics in dependency of the excitation wavelength are of vital interest. Up to now, polaron excitation has been investigated in the vis-spectral range via two-photon absorption (TPA) whereas polaron dynamics initiated by higher photon energies are largely unknown.

We have addressed this question by performing systematic studies under deep UV-pulse excitation at 355 nm and probed with different cw-lasers via transient absorption spectroscopy. Optical excitation and recombination of small polarons is analyzed in terms of pump-intensity and temperature in congruent, Mg-, and Fe-doped lithium niobate (LN). At 355 nm, the bound/free polaron formation probability for congruent and Mg-doped LN increases towards the UV region because of a growing TPA coefficient, whereas iron-doped LN exhibits a decreased bound polaron formation probability altogether compared to an excitation at 532 nm due to an altered excitation path. Latter can be explained by a single photon absorption (SPA) from the valence band into the Fe^{3+}-state forming hole-polarons and Fe^{2+}. Furthermore, SPA quenches TPA and therefore, band to band transitions are suppressed. Financial support by the DFG (IM 37/5-2, INST 190/165-1 FUGG) is gratefully acknowledged.

KFM 27.12 Thu 15:00 Poster E

Surface acoustic wave propagation in monoclinic ferroelectric phases in strained $K_{0.7}Na_{0.3}NbO_3$ thin films — •Jutta Schwarzkopf[1], Leonard von Helden[1], Sijia Liang[2], Roger Wördenweber[2], and Martin Schmidbauer[1] — [1]Leibniz Institute for Crystal Growth, Max-Born-Str. 2, Berlin, Germany — [2]Peter Grünberg Institute, Forschungszentrum Jülich, Jülich, Germany

Formation of ferroelectric phases with monoclinic symmetry is expected to result in enhanced piezoelectric properties. Together with high coupling coefficients, this feature can be exploited for thin film surface acoustic wave (SAW) devices. $K_xNa_{1-x}NbO_3$ represents a suitable material system that does not only provide high coupling coefficients. In addition, monoclinic phases can be stabilized in thin films

by applying anisotropic epitaxial strain. Though as known from previous studies [1], the formation of the monoclinic phase crucially depends on the incorporated lattice strain. In this work, 30 nm $K_{0.7}Na_{0.3}NbO_3$ films were grown epitaxially on (110) $TbScO_3$ and (110) $GdScO_3$ substrates by metal-organic chemical vapor deposition. The films exhibit a compressive strain state with pseudocubic $(001)_{pc}$ surface orientation and periodically arranged ferroelectric stripe domains. Piezoresponse force microscopy and x-ray diffraction reveal a domain periodicity of $40 - 50$ nm and domains walls that proceed along the $[11\overline{2}]$ or $[1\overline{1}\overline{2}]$ directions of the orthorhombic substrates. These films were used for SAW experiments. Differences in SAW propagation will be discussed with regard to the symmetry of different monoclinic phases.

[1] J. Schwarzkopf et al., Front. Mater. 4, 26 (2017)

KFM 27.13 Thu 15:00 Poster E

Wavevector dependent optical properties from wavevector independent ab initio conductivity tensor — •René Wirnata[1], Ronald Starke[1], Giulio Schober[2], and Jens Kortus[1] — [1]Institut für Theoretische Physik, TU Bergakademie Freiberg — [2]Institut für Theoretische Festkörperphysik, RWTH Aachen

In ab initio materials physics it is common practice to consider the conductivity tensor $\sigma(\boldsymbol{k},\omega)$ in the optical limit, i.e. $\boldsymbol{k} \to \boldsymbol{0}$. However, response functions are naturally functions of both wavevector and frequency. Using *Universal Response Relations* [1], we are able to construct e. g. a frequency and wavevector dependent dielectric tensor from a wavevector independent optical conductivity. Since the dielectric function and the refractive index are related by $n^2 = \varepsilon$, we can thus calculate ab initio ordinary and extra ordinary refractive indices, $n_e(\omega)$ and $n_o(\omega)$, of birefringent materials that fit very well with experimental results from [2]. In fact, obtaining the scalar functions $n_e(\omega)$ and $n_o(\omega)$ from a dielectric tensor $\varepsilon(\boldsymbol{k},\omega)$ requires in the most general case a more sophisticated algorithm, which is already known in theoretical optics [3-4]. In order to illustrate the reliability of this approach for different materials types, we have chosen Si, TiO_2 and α-Quartz as examples for isotropic, birefringent and optically active crystals.

[1] R. Starke, G.A.H. Schober: Photonic.Nanostruc. **14** (2015)
[2] E. Palik: Handbook of Optical Constants of Solids (2002)
[3] H. Römer: Theoretische Optik, Wiley-VCH (1994)
[4] R. Starke, G.A.H. Schober: arXiv:1708.06330

KFM 27.14 Thu 15:00 Poster E

Construction of a broadband Sub-THz-Spectrometer — •Max Pargmann, Christoph Grams, and Joachim Hemberger — Universität zu Köln

Between the highest frequencies that are accessible with conventional dielectric spectroscopy (≈2E10 Hz) and the lowest in optical free-beam spectroscopy (≈2E11 Hz), measurements are difficult due to technical limitations [1]. We try to close this frequency gap by building a new time-domain spectrometer enabling us to measure a wide frequency range starting from 5 GHz up to 500 GHz. We use a pulsed laser setup with a variable delay up to 500 ps combined with a pulse picker to customize the average optical power. For measurement, we use an on-chip emitter detector design in microstrip geometry, with embedded GaAs photoconductive switches, which allows for generation and detection of pulses ≈ 300 fs [2]. The spectrometer is compact and complete fiber based therfore it can be easily implimentated in commerical magneto cryostats without the need of free beam.

This work is supported by the Deutsche Forschungsgemeinschaft via SFB1238 (Cologne).

[1] C. Matheisen et al, IEEE Xplore 15598877(2015)
[2] M.B. Byrne et al, Appl. Phys. L93, 182904 (2008)

KFM 27.15 Thu 15:00 Poster E

Optimising interferometric displacement detection for NC-AFM operation — •Alexander von Schmidsfeld and Michael Reichling — Universität Osnabrück

We systematically describe the steps needed for optimal calibration of interferometric displacement detection of the cantilever in NC-AFM and demonstrate that the interferometer for displacement detection can be operated in both, the Michelson and the Fabry-Perot mode. After describing the basic interferometer setup, we present a method to characterize the optical losses occurring in the feed line and the results of deficient fiber-cantilever alignment. Furthermore, we introduce the method of 3D intensity mapping of the optical cavity response and recordings of the interferometer signal as a function of the fiber-end-to-cantilever distance, both together allowing us to optimize the adjustment. Finally we examine the impact of opto-mechanical effects occurring in a cavity of sufficient finesse on the detection noise figures and the effective parameters of the cantilever oscillation, namely the Q-factor Q0 and the stiffness k0, both split into values for positive and negative fringes of the interferogram, respectively.

KFM 27.16 Thu 15:00 Poster E

Limitations of Single-Step Phase Retrieval — •Johannes Hagemann[1,2], Mareike Töpperwien[1], and Tim Salditt[1] — [1]Institut für Röntgenphysik, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]current address: DESY, X-Ray Nanoscience and X-Ray, Optics, Notkestraße 85, 22607 Hamburg

In order to harness the full information of propagation-based phase contrast images obtained with coherent x-rays, one has to carry out a phase reconstruction on the images. This strategy is applied for data obtained in various optical regimes ranging from the edge enhancement to the deeply holographic regime.

By placing assumptions on the specimen e.g. weak absorption one can construct several single-step solutions for the respective optical regime. Despite the merrits of these schemes, the reconstruction obtained is only as good as the assumptions hold.

We demonstrate on an example near-field hololographic dataset, the flaws of the single-step reconstruction based on the contrast transfer function[1] and the possible improvement gained by applying an iterative reconstruction scheme.

[1] P. Cloetens et al., Appl. Phys. Lett.(1999), **75**, 2912*2914.

KFM 27.17 Thu 15:00 Poster E

In situ gas-cell for the analysis of sorption behavior on surfaces by using X-ray fluorescence and absorption spectrometry under total reflection geometry — •Cornelia Streeck[1], Daniel Grötzsch[2], Jan Weser[1], Wolfgang Malzer[2], Andreas Nutsch[3], Thomas Wiesner[1], Birgit Kanngiesser[2], and Burkhard Beckhoff[1] — [1]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin, Germany — [2]Technische Universität Berlin and Berlin Laboratory of innovative X-ray Technologies, Hardenbergstr. 36, 10623 Berlin, Germany — [3]Helmut Fischer GmbH, Industriestraße 21, 71069 Sindelfingen

A novel measuring cell for in-situ metrology of molecules of light elements e.g. volatile organic compounds and their sorption behavior on different surfaces was developed. The cell is designed for the soft X-ray range (especially C, N, and O) and is constructed for flow-through operation in a high-vacuum chamber. It allows for the analysis of the surface under total reflection geometry with Total-Reflection X-Ray Fluorescence (TXRF) analysis and X-ray Absorption Spectroscopy (XAS). First experiments using ethanol on steel and Si-wafer surfaces were applied.

KFM 27.18 Thu 15:00 Poster E

Detection of electronic anisotropies in cuprates by precision x-ray polarimetry with quartz crystals — •Annika Tamara Schmitt[1,2], Ingo Uschmann[1,2], Kai Sven Schulze[1,2], Robert Lötzsch[1,2], Hendrik Bernhardt[1,2], Benjamin Grabiger[1,2], Berit Marx-Glowna[2,3], Yves Joly[4], Martin von Zimmermann[3], Hasan Yavas[3], Hans-Christian Wille[3], Eckhart Förster[2], Gerhard Paulus[1,2], and Ralf Röhlsberger[3] — [1]Institut für Optik und Quantenelektronik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, D-07743 Jena, Germany — [2]Helmholtz-Institut Jena, Helmholtzweg 4, D-07743 Jena, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, D-22607 Hamburg, Germany — [4]Institut Néel , 25 Avenue des Martyrs, F-38042 Grenoble, France

To understand the origin of the high-temperature superconductivity in the cuprates, it is necessary to study the electronic structure of the copper oxides. Information about the electronic structure and symmetry can be obtained by XANES measurements at the Cu K-edge. The combination of x-ray spectroscopy and x-ray polarimetry offers a much more sensitive method to explore electronic anisotropies and magnetic moments, since the absorption depends on the polarization state.Using crossed x-ray polarizers, tiny optical anisotropies caused by electronic anisotropies can be detected. The x-ray polarizers are based on Bragg reflection at scattering angles very close to 90°. Polarization purities up to $1.2 \cdot 10^{-7}$ can be reached using quartz polarizers with a 320-reflection at the Cu K-edge.

KFM 27.19 Thu 15:00 Poster E

XAFS by an X-ray tube based laboratory spectrometer — •Sebastian Praetz[1], Christopher Schlesiger[1], Lars

Anklamm[1,3], Holger Stiel[2], Wolfgang Malzer[1], and Birgit Kanngiesser[1] — [1]Institute for Optics and Atomic Physics, Technical University Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Max-Born-Insitut, Max Born-Straße 2a, 12489 Berlin, Germany — [3]IAP e.V., Rudower Chaussee 29/31, 12489 Berlin, Germany

The spectroscopy of X-ray Absorption Fine Structure (XAFS) is a frequently used method for the investigation of the electronic structure or for the identification of chemical compounds, such as the oxidation state or coordination of functionalized materials. This technique is usually performed at synchrotron radiation facilities because of the need of a brilliant X-ray source and a high spectral resolving power. A laboratory setup would have the advantage of higher accessibility and flexibility, which would open this technique for routine analysis.

In this contribution, we will present our successfully developed X-ray tube based von Hamos laboratory XAFS spectrometer using a novel type HAPG mosaic crystal with a spectral resolving power up to $E/\Delta E = 4000$ and a wide energy range of 4 keV to 12 keV.

We are able to measure liquid as well as solid state samples in transmission. Usual acquisition times are in the range of a few minutes to several tens of minutes. First applications will be shown, e.g. the identification of oxidation states. These results are very promising and show the capability of this spectrometer for all kinds of XAFS measurements.

KFM 27.20 Thu 15:00 Poster E

3D reconstruction from one-dimensionally blurred projections — •Leon Merten Lohse, Malte Vassholz, and Tim Salditt — Institut für Röntgenphysik, Friedrich-Hund-Platz 1, 37077 Göttingen, Deutschland

Although high-brilliance radiation sources become more and more available, many applications are depending on laboratory x-ray sources or neutron sources with low brilliance. Due to the low brilliance, a trade-off between high resolution and feasible acquisition time has to be made. The use of 1D (line) sources has been demonstrated recently, to be able to increase the flux without any impact on the resolution and thus circumvent the trade-off [1,2]. A particularly simple method, which is based on the 3D Radon transform, can be used to reconstruct the 3D volume from a set of projections from a line source. If the divergence of the beam can be neglected, the planar integrals required for the 3D Radon transform can be directly extracted from the projections, and a 3D analogon to the well-known filtered-back-projection algorithm can be formulated.

[1] L. M. Lohse et al. "Tomography with extended sources: ...", Phys. Rev. A (accepted 11/2017) [2] M. Vassholz et al. "New X-Ray Tomography Method ... ", Phys. Rev. Lett. (2016)

KFM 27.21 Thu 15:00 Poster E

X-ray emission spectroscopy (XES) by an X-ray tube based laboratory spectrometer — •Richard Gnewkow[1], Christopher Schlesiger[1], Daniel Grötzsch[1], Lars Anklamm[2], Fabian Kowalewski[3], Serena DeBeer[3], Wolfgang Malzer[1], and Birgit Kabbgiesser[1] — [1]Institute for Optic and Atomic Physics, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Institut für angewandte Photonik e. V. (IAP), Rudower Chaussee 29/3, 12489 Berlin, Germany — [3]Max Planck Institute for Chemical Energy Conversion, Stiftstr. 34 - 36, 45470 Mülheim a.d. Ruhr, Germany

X-ray emission spectroscopy (XES) is an upcoming method for the investigation of the electronic structure of chemical compounds. Typically the chemical shift of the Kβ-multiplett is analyzed. XES, therefore, requires a high spectral resolution and is mainly performed at synchrotron facilities.

We developed an X-ray tube based laboratory spectrometer for XES experiments. The dispersive element is a graphite mosaic crystal called Highly Annealed Pyrolytic Graphite (HAPG) in an adapted von Hamos geometry. The full cylinder optic combines high efficiency with a spectral resolving power of $E/\Delta E = 4000$ for an energy range between 2 keV - 10 keV. The use of a polycapillary lens allows the analysis on a micrometer scale.

In this contribution, we will present the setup of the spectrometer and its properties. We will show results for the Kβ diagram line and valence-to-core region for thin and diluted samples, e.g. catalysts.

KFM 27.22 Thu 15:00 Poster E

X-ray fluorescence and X-ray diffraction analysis of a historical painting — •Fatima Mallal[1], Alex von Bohlen[2], Christian Sternemann[1], Michael Paulus[1], Anne Hüsecken[1], Paul Salmen[1], Wolf-Dieter Köster[3], Jörg Hansen[4], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, Technische Universität Dortmund, Germany — [2]Leibniz-Institut für Analytische Wissenschaften ISAS, Germany — [3]Dortmund, Germany — [4]Bachhaus Eisenach, Germany

According to the current state of knowledge, there are only two paintings of Johann Sebastian Bach (1685-1750) which were made during his life time. Both are exhibited in the *Bach House* in Eisenach. We present an X-ray fluorescence (XRF) and X-ray diffraction (XRD) study on a third painting of unspecified origin in order to proof its authenticity, which was performed at beamline BL 9 of DELTA synchrotron radiation source. The XRF data was used to detect the elemental composition of the painting, whereas the XRD pattern provide insight into the crystal structure of colors and pigments. This analysis enables to draw conclusions about the age of the painting, as specific colors are characteristic for certain ages.The XRF analysis showed a predominant contribution of the elements lead, zinc, calcium and barium. We identified the pigments lead white (2PbCO3 Pb(OH)2), lithopone (BaSO4 ZnS), and low amount of zinc white (ZnO) at different regions of the painting. Moreover chalk (CaCO3) was detected. The observation of the different pigments indicates that corrections of the portrait have been made in the 19th century.

KFM 27.23 Thu 15:00 Poster E

Harmonic nanoparticles as markers for in-vivo imaging — •Dustin Dzikonski[1], Christian Kijatkin[1], Kay Lammers[2], Achim Paululat[2], and Mirco Imlau[1] — [1]Department of Physics, Osnabrück University, Germany — [2]Department of Zoology & Developmental Biology, Osnabrück University, Germany

Nanoscaled optical markers are versatile contrast agents in biological environments; especially fluorescing dyes have risen to a microscopy standard. However, rather rigid excitation-emission wavelengths as well as Stokes shifts towards the red spectrum pose severe limitations to this class of materials. Moreover, time-critical analysis is hindered due to photobleaching, blinking, and potentially long fluorescent lifetimes.

A solution is the use of harmonic, alkali niobate-based nanoparticles that offer unprecedented flexibility due to their photostability, instantaneous response, and frequency tunability in a vast range [C. Kijatkin *et al.*, *Photonics* **2017**, *4*(1), 11]. In light of novel applications, we plan to utilize infrared radiation from femtosecond pulsed lasers in combination with harmonic generation to i) increase excitation depth due to the lower absorption in this range, ii) create visible up to UV light for detection and manipulation, and iii) allow for time-critical evaluation of dynamic systems. As a proof of principle, we present our studies on using lithium niobate nanoparticles as tracers via second harmonic generation of infrared radiation to visualize and quantify the hemolymph velocity flux inside the heart chamber of living *Drosophila melanogaster* as a model system. Financial support (DFG INST 190/165-1 FUGG) is gratefully acknowledged.

KFM 27.24 Thu 15:00 Poster E

Ptychography goes magnetic: Developing direct magnetic imaging with hard X-rays at PETRA III's P09 — •Florian Heinsch[1,2], Felix Wittwer[3], Sonia Francoual[3], Dennis Brückner[3], Maik Kahnt[3], Martin Seyrich[3], David Reuther[3], Martin Zwiebler[2], and Jochen Geck[2] — [1]HZDR, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]DESY, Hamburg, Germany

X-rays are an ideal probe for non-destructive imaging of a bulk-sample's structure, featuring high spatial resolution and possible element sensitivity. Our goal is to combine these properties with the magnetic sensitivity provided by the X-ray absorption process in order to image magnetic properties with nanometer resolution.

We present the results of a first experiment at the magnetic scattering beamline P09 of PETRA III. All additionally required components, including focusing lenses, could be successfully integrated in the beam path with a stability that allowed for conventional ptychography with a resolution of at least 60nm. Subsequently it will be possible to directly map out the XMCD of a given thin sample. Therefore the difference of two ptychograms with opposing circularly polarized light needs to be compared. First results are presented and an outlook is given on the way to imaging of magnetic domains by magnetic ptychography at PETRA III.

KFM 27.25 Thu 15:00 Poster E

Analysis of Multilayer Zone Plates (MZP) for Imaging with

hard X-Rays and Nanometer Resolution — •Jakob Soltau, Lars Melchior, Tim Salditt, and Markus Osterhoff — Institut für Röntgenphysik, Georg-August-Universität Göttingen, Göttingen, Germany

The brilliance of modern synchrotrons cleared the path towards generating highly focussed x-ray beams. While focal spot diameters of a few nanometers are already common at lower x-ray energies (< 10 keV), there is a lack of x-ray optics suited for scanning microscopy with small spot sizes at higher energies. The challenge for manufacturing zone plates in the hard x-ray energy range is the high aspect ratio, defined by the large optical thickness (>5 μm) - needed due to the low interaction between photons and matter - and small zone widths (<10 nm) [1]. The propagation of electromagnetic waves in structures not much larger than their wavelength and with high-aspect ratios lead to effects as waveguiding and dynamical diffraction. To assess these effects and characterize the efficiency of multilayer zone plates (MZP) 3D finite-differences simulations [2] have been performed. The simulation of the electromagnetic fields inside and behind the MZP showed the advantage of circular MZPs to achieve very high photon flux densities in a single focal point of 5 nm diameter. Furthermore the simulations were revealing interaction processes like e.g. dynamical diffraction inside the MZPs. [1] C. Eberl et al. Fabrication of laser deposited... In: Applied surface science 307 (2014) [2] L. Melchior et al. Finite difference methods for... In: Opt. Express (accepted)

KFM 27.26 Thu 15:00 Poster E

DLTPulseGenerator: A C/C++ Library for the Simulation of Lifetime-Spectra based on Detector-Output Pulses — •Danny Petschke and Torsten Staab — University Würzburg, Dep. of Chemistry, LCTM, Röntgenring 11, D-97070 Würzburg, Germany

The quantitative analysis of lifetime spectra relevant in both life- and material sciences presents one of the ill-posed inverse problems and, hence, leads to most sophisticated requirements on the hardware-specifications and -parameters of the setup as well as on the analysis algorithms. Here we present DLTPulseGenerator, a library written in native C++ 11 which provides a simulation of lifetime spectra according to the measurement setup: i.e. the kind of detectors and the acquisition hardware. The simulation is based on pairs of non-TTL detector-pulses. Those pulses require the Constant-Fraction Principle (CFD) for the determination of the exact timing signal and, thus, the calculation of the time difference i.e. the lifetime. The library provides the simulation of discrete specific lifetimes (e.g. metals, polymers) and the simulation of specific lifetime distributions (Gaussian, Lorentzian and Log-Normal) as can be found in porous materials, i.e. Vycor-glasses and aerogels. To verify our method, simulation results were visually and quantitatively compared to experimentally obtained data using Positron-Annihilation Lifetime Spectroscopy (PALS) on pure Aluminium (4N).

KFM 27.27 Thu 15:00 Poster E

Quantum electronic scattering in a Au/Co/Au nanowire lead — Adel Belayadi[1] and •Boualem Bourahla[2] — [1]University of M. Bougara, Department of Coating Material and Environmental, Boumerdes, Algeria — [2]Laboratory of Physics and Quantum Chemistry, M. Mammeri University, Tizi-Ouzou, Algeria

In the present contribution, we provide a theoretical model to investigate the electron scattering states in a one-dimensional atomic chain which contains a single defect atom. In fact, in ideal leads the translation symmetry is treated by periodic boundary conditions. However, in the case of a defect, the Bloch theorem is not applicable. In other words, the single defect atom breaks the symmetry and makes the solution of eigenvalues problem impossible. To deal with inhomogeneous systems, due to lack of symmetry, we have integrated the phase field matching theory (PFMT) to compute the eigenvalue problem of our system. The PFMT connects the left and right leads, separated by the defect atom, in terms of the total transmission and reflection probabilities of the Landauer-Büttiker formalism. As application, we build up the Hamiltonian matrix in the tight-binding approach and then we compute the coherent scattering and transport of electron as well as the electronic conductance across the defect junction given as copper/cobalt/copper, while the cobalt atom is treated as a defect atom.

KFM 27.28 Thu 15:00 Poster E

High-resolution structural and chemical analysis of transition metal oxide nanoparticles — •Aladin Ullrich, Daniel Schmidtner, Mohammad Mostafizar Rahman, and Siegfried Horn — University of Augsburg, 86159 Augsburg, Germany

We have investigated the structural and chemical composition of pure iron oxide and manganese ferrite nanoparticles by transmission electron microscopy (TEM). The particles were synthesized by thermal decomposition of the corresponding metal oleate salts in high-boiling solvents. Na-oleate was used as surfactant for shape control during the synthesis.

The synthesized particles are 20nm in size and appear core-shell like in bright field TEM images. High-resolution TEM (HRTEM) analysis reveals a FeO/MnO like structure in the core and a spinel like structure in the shell.

To resolve the spatial distribution and the oxidation state of the metals manganese and iron within the particles, high-resolution energy loss spectroscopy (EELS) and energy dispersive x-ray spectroscopy (EDS) were performed.

Iron and manganese show differences between their oxidation state in the core and the shell region of the particles. This is consistent with the structures observed in HRTEM analysis. The oxidation state of the iron ions is lower in the core than in the shell region. For manganese ions, only a thin surface layer shows different oxidation state. Traces of sodium used as surfactant during the synthesis were detected on the surface of the particles.

KFM 27.29 Thu 15:00 Poster E

Electro-osmotic pumping for structured coatings — •raheema muhammad aslam, Ran Niu, and Thomas Palberg — Institute of Physics, JGU Mainz, Germany

We assemble charged colloidal spheres at deliberately chosen locations on a charged unstructured glass substrate utilizing ion exchange based micro-pumps. The pump uses trace amounts of ions to generate electro-osmotic fluid flows. We show experimentally that our pump operates in almost deionized water for periods exceeding 24 h and induces fluid flows in micrometer per second over hundreds of micrometers. This flow displays a far-field, power-law decay which is characteristic of two-dimensional (2D) flow when the system is strongly confined and of three-dimensional (3D) flow when it is not. Experimentally, we systematically explore the control parameters of crystal assembly at and by micro-pumps and the mechanisms through which they depend on the experimental boundary conditions. We demonstrate that crystal quality depends crucially on the assembly distance of the colloids. This is understood as resulting from the competition between inward transport by the electro-osmotic pump flow and the electro-phoretic outward motion of the colloids. Optimized conditions include substrates of low and colloids of large electro-kinetic mobility. Then a sorting of colloids by size is observed in binary mixtures with larger particles assembling closer to the ion exchanger beads. Moreover, mono-sized colloids form defect free single domain crystals which grow outside a colloid-free void with facetted inner crystal boundaries centred on the ion exchange particle.

KFM 27.30 Thu 15:00 Poster E

Cladding-like waveguide structure in Nd:YAG crystal fabricated by multiple ion irradiation for enhanced waveguide lasing — •zhen shang[1,2], shengqiang zhou[1], and yang tan[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]School of Physics Shandong University, Jinan, China

we report on a cladding-like waveguide structure in Nd:YAG crystal fabricated by the multiple carbon ion beam irradiation. After the designed multiple irradiation process, the cladding-like waveguide with triple refractive-index layers were constructed in the region near the surface of the crystal. With such a structure, the waveguiding core was compressed and refractive index profile was modified, resulting in a higher light intensity than that of the single ion-beam-irradiated monolayer waveguide. The waveguide lasing at wavelength of 1064 nm was achieved with enhanced performance in the cladding-like structures with both planar and ridge configurations by the optical pump at 810 nm.

KFM 27.31 Thu 15:00 Poster E

Crystallisation of Bismuth in an Inert Atmosphere and Electrical Characterization of these Crystals — •Christian Düputell, Arne Ludwig, and Andreas D. Wieck — Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstraße 150, D-44780 Bochum

The aim of this work is to validate diverse melting processes for the

growing of bismuth crystals in different gas atmospheres (purity of used Bi: 99,99%). Therefore, melting in two different atmospheres has been performed; in air and in an inert atmosphere (argon). The methods were assessed in terms of characterisation of the grown crystals; for this purpose, the crystals were examined visually as well as electrically.
A particular advantage of an inert atmosphere is the prevention of oxidation of the growing crystals. This leads to the formation of purer, larger as well as more distinct bismuth crystals. The observation has been proven in two different ways: first by a visual characterisation of the crystals using a light microscope and second by Hall-Effect measurements of selected crystal samples. The results of the Hall-Effect measurements demonstrate the particular electrical and magnetic properties of the half-metal bismuth. At room temperature, the measured Hall-coefficient of crystals formed in the air is about $-9,64(30) \cdot 10^{-9}$ m^3 C^{-1} in comparison to $-9,42(16) \cdot 10^{-7}$ m^3 C^{-1} of crystals formed in an inert atmosphere.
Furthermore, a modification of the so called "Czochralski process" has been examined. So in future works it may be possible to improve the forming of bismuth single crystals without manual intervention.

KFM 27.32 Thu 15:00 Poster E

The Influence of Rare Earth Doping and Co-doping of ZnO Nanoparticles on Structural and Optical Properties — •Maria Toma[1,2], Oleksandr Selyshchev[3], Aurel V. Pop[1], and Dietrich R.T. Zahn[3] — [1]Babes-Bolyai University, Physics Faculty, M. Kogalniceanu No. 1, 400084, Cluj-Napoca, Romania — [2]Research Center for Advanced Medicine Iuliu Hatieganu University of Medicine and Pharmacy, Cluj-Napoca, Romania — [3]Chemnitz University of Technology, Semiconductor Physics, D-09107 Chemnitz, Germany

Gd-doped, Er-doped, and (Gd+Er) co-doped ZnO nanocrystals were prepared by a soft colloidal synthesis method [1]. Due to their applications in optoelectronic, display, and memory devices [2,3], semiconductor nanocrystals doped with rare earths (RE) are of great interest. Microstructural properties of the nanocrystals obtained were characterized using Raman spectroscopy and their distribution and crystallinity were identified using transmission electron microscopy. From TEM measurements we evaluated the size of the nanoparticles to be in the range of 4 to 7 nm. Optical properties were investigated using photoluminescence (PL) and UV-vis spectroscopy to understand the excited state energy distribution between band to band transitions and the defect states. Depending on the size distribution of the nanoparticles, changes in the PL and UV absorbance of ZnO were observed, due to the incorporation of RE ions into the ZnO nanostructure Owing to the electronic configuration of the RE ions, the 4f shell transitions show sharp and narrow band emission. This effect is consistent with Raman and other literature results.

KFM 27.33 Thu 15:00 Poster E

Discovery of a high-pressure RuCl3 phase with complete cation disorder — •Lisa Leissner, Ulrich Bläss, Marcus Schwarz, and Edwin Kroke — Tu Bergakademie Freiberg, Freiberg, Germany

The alpha form of Ruthenium(III)-chloride is a hot topic in spin liquid physics because it is one of the most promising materials to realize the Kitaev model of a quantum spin liquid. It fulfills the criteria for realizing the Kitaev interactions (Jackeli & Khaliullin 2009, Glamazda et al 2017). At low temperatures, it orders to a zigzag magnetic order. However, in Raman spectroscopy as well as inelastic neutron scattering some hints of spin liquid physics could be observed (Sears et al, 2017). The transition temperature is strongly dependent of the sample, especially its stacking faults. The effective magnetic interactions between the Ru-moments strongly depend on the distance and Ru-Cl-Ru angle. Hence, a change of one of these parameters, as e.g. occurring after second order phase transitions, may change the ratio between Kitaev and Heisenberg interactions. In order to explore such potential transitions, we have conducted various heated and unheated high pressure experiments to explore stable or metastable high-pressure phases of RuCl3. Multianvil experiments led to the formation of single crystals of a new RuCl3 phase. Single crystal X-ray diffraction revealed a small unit cell with space for two atom sites only, while spectroscopic measurements indicate that a Ru:Cl ratio of 1:3 is still present. We thus have synthesized a new and possibly metastable hexagonal form of RuCl3 with a completely random occupation of one third of the cation site.

KFM 27.34 Thu 15:00 Poster E

Single-crystal diffractometers HEiDi and POLI at MLZ: (Un)polarised neutrons to probe crystallographic and magnetic domains — •Andrew Sazonov[1,2], Martin Meven[1,2], Vladimir Hutanu[1,2], and Georg Roth[1] — [1]RWTH Aachen, Institute of Crystallography, D-52056 Aachen, Germany — [2]Jülich Centre for Neutron Science at MLZ, D-85748 Garching, Germany

HEiDi and POLI are the only single-crystal neutron diffractometers in Germany and two of the very few in the world which are located at a hot neutron source to enlarge the flux of neutrons with short wavelengths. It allows to minimize the absorption problems associated with certain elements and to explore extremely large portions of reciprocal space. HEiDi is a typical 4-circle diffractometer with Eulerian cradle for detailed studies on crystal and magnetic structures in the temperature range 2.5–1300 K. POLI is an independent diffractometer, which extends the possibilities of HEiDi to the milli-Kelvin range and external magnetic fields as well as offers in addition different types of polarized neutron techniques: Flipping-ratio measurements in applied magnetic field for ferromagnetic and paramagnetic materials and spherical neutron polarimetry in zero field for more complex magnetic structures. Due to their possibilities, both instruments contribute to many topics, e.g. in the energy and information sector. Here, on examples of multiferroic and superconducting materials, we give an overview of the instruments possibilities in studying of crystal and magnetic structures and phase transitions of solids in general, and their crystallographic and magnetic domains (microstructures) in particular.

KFM 27.35 Thu 15:00 Poster E

The crystal structure of trisodium hexachloroiridate — •Martin Etter[1], Melanie Müller[2], and Sebastian Bette[3] — [1]Deutsches Elektronen-Synchrotron, Hamburg, Germany — [2]Universität Duisburg-Essen, Duisburg, Germany — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

Strongly hygroscopic inorganic compounds exhibit a rich field of unsolved crystal structures as often several hydrated forms exist. However, solving these crystal structures is challenging, since single crystals are in many cases not available and powders usually consist of several hydrated phases at the same temperature and moisture conditions. Such a challenging compound is for instance the highly hygroscopic trisodium hexachloroiridate (Na3IrCl6) which possess multiple hydrated phases and a so far unsolved crystal structure even of the anhydrous phase.

Here, the crystal structure of the anhydrous phase of trisodium hexachloroiridate (Na3IrCl6) at room temperature was solved after a dehydration process using laboratory powder X-ray diffraction. It was found that the crystal structure of Na3IrCl6 crystallizes in space group P-31c isostructural to the crystal structures of Na3CrCl6, Na3InCl6 and Na3MoCl6 as well as to recently found crystal structure of trisodium hexachlororhodate (Na3RhCl6).

In this presentation structural details about the dehydrated compound will be given as well as an outlook to the variety of hydrated phases.

KFM 28: Complex Oxides: Bulk Properties, Surfaces and Interfaces (joint session TT/MA/KFM)

Time: Friday 9:30–13:00 Location: H 0110

KFM 28.1 Fri 9:30 H 0110

Superconductivity in strontium titanate within the dielectric function method — •Serghei Klimin[1], Jacques Tempere[1], Jozef Devreese[1], Cesare Franchini[2], and Georg Kresse[2] — [1]TQC, Universiteit Antwerpen, Antwerpen, Belgium — [2]University of Vienna, Faculty of Physics and Center for Computational Materials Science, Vienna, Austria

Strontium titanate exhibits unique features which are not encountered in conventional polar crystals at the same conditions. It becomes a superconductor at unusually low carrier densities. $SrTiO_3$ is probably the only substance where superconductivity and optical absorption can be convincingly attributed to the Fröhlich-like electron-phonon interaction and polarons. In the present talk, we report on our theoretical studies of superconductivity in strontium titanate with a comparative discussion of different theoretical interpretations of superconductivity in $SrTiO_3$. It is demonstrated that the dielectric function method used in our works [1] adequately describes the superconducting phase transition using only parameters available from experiments and microscopic calculatuions. We are particularly focused on unusual isotope effect in $SrTiO_3$. It is shown that renormalization of optical-phonon frequencies following from the isotope substitution leads to an increase of the critical temperature within the dielectric function method.
[1] S. N. Klimin, J. Tempere, J. T. Devreese, and D. van der Marel, Phys. Rev. B **89**, 184514 (2014); J. Sup. Nov. Magn. **30**, 757 (2017).

KFM 28.2 Fri 9:45 H 0110

Anisotropic Rashba-type spin-orbit coupling of the two-dimensional electron system in (110) $SrTiO_3$-based heterostructures — •Karsten Wolff, Roland Schäfer, Robert Eder, Matthieu le Tacon, and Dirk Fuchs — Karlsruhe Institute of Technology, Institute for Solid State Physics

The two-dimensional electron system in (110) $Al_2O_{3-d}/SrTiO_3$ heterostructures displays anisotropic electronic transport. Structured microbridges allow to probe 4-point resistivity along different crystallographic orientations, i.e. [001] and [1-10]. The conductivity and electron mobility along the [001] direction is largest, while differences in sheet carrier concentration are only minor. The measurements show anisotropic normal magnetotransport for $T < 30\,K$ which is correlated to the anisotropic mobility. For temperatures below 5 K transport is dominated by Rashba-type spin orbit interaction (SOI) which displays anisotropic behavior, too. SOI is found largest along the [001] direction.

KFM 28.3 Fri 10:00 H 0110

Thermoelectric properties of $(SrXO_3)_1(SrTiO_3)_m$(001) superlattices, X=V, Mn and Ru — •Manish Verma, Benjamin Geisler, Markus E. Gruner, and Rossitza Pentcheva — Department of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, 47057 Duisburg

The thermoelectric properties of $SrTiO_3$ have been widely studied, primarily concerning the role of homogeneous bulk doping. However, the confinement realized in oxide superlattices may have a favorable effect on the thermoelectric properties. To this end we have investigated the electronic and thermoelectric properties of superlattices containing a monolayer of $SrXO_3$ (X=V, Mn and Ru) sandwiched between m=1,3 spacer layer(s) of $SrTiO_3$ (001) using a combination of density functional theory with an on-site Hubbard term and semi-classical Boltzmann theory. In all cases structural distortions containing octahedral tilts are energetically favored over tetragonal distortions and we explore their influence on the electronic and thermoelectric properties. Comparing the in-plane and out-of-plane transport properties we find no significant dependence on m for the in-plane transport properties. In turn on reduction of the $SrTiO_3$ thickness from m=3 to 1 enhances the dispersion along Γ-Z and thereby improves the out-of-plane thermoelectric properties. Funded by the DFG, CRC/TRR80 project G8.

KFM 28.4 Fri 10:15 H 0110

Thermoelectricity close to a metal-insulator transition in ultrathin $LaNiO_3/LaAlO_3$(001) superlattices — •Benjamin Geisler and Rossitza Pentcheva — Fakultät für Physik, Universität Duisburg-Essen, 47057 Duisburg, Germany

Transition metal oxides are a promising materials class for thermoelectric applications due to their chemical and thermal stability and environmental friendliness. Their thermoelectric response can be further improved by nanostructuring and reduced dimensionality. Here we explore the thermoelectric properties of $(LaNiO_3)_1/(LaAlO_3)_1$(001) superlattices near the confinement-induced metal-insulator transition by combining *ab initio* simulations including on-site Coulomb repulsion and Boltzmann theory. We find that the short-period vertical design strongly enhances the in-plane thermoelectricity owing to the Ni-site disproportionation, which is stabilized considerably by tensile epitaxial strain and octahedral tilting. The sensitivity of the system to epitaxial strain provides an additional parameter to optimize the thermoelectric performance. For a $SrTiO_3$(001) substrate, we predict room-temperature Seebeck coefficients and power factors that can compete with those of other oxide systems of current interest such as layered cobaltates. Comparison of the ultrathin superlattices with the metallic longer-period $(LaNiO_3)_3/(LaAlO_3)_3$(001) case establishes the metal-insulator transition as a crucial mechanism to obtain a high thermoelectric response.

Funding by the DFG within TRR 80 (G3 and G8) is acknowledged.

KFM 28.5 Fri 10:30 H 0110

Confinement-driven electronic and topological phases in corundum-derived oxide honeycomb superlattices — •Okan Koeksal and Rossitza Pentcheva — Department of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, 47057 Duisburg

On the basis of density functional theory calculations plus the Hubbard U interaction, we investigate electronic, magnetic and possibly topologically non-trivial phases in X_2O_3 honeycomb layers confined in the corundum structure α-Al_2O_3 (0001). Our results predict that the ground states for most of the systems of $X = 3d$ cations are trivial antiferromagnetic Mott insulators. If the symmetry of the two sublattices is imposed, the ferromagnetic phases of Ti, Mn, Co and Ni exhibit a characteristic set of four bands associated with the single occupation of e'_g (Ti) and e_g (Mn, Co, Ni) states. Moreover, the Dirac point can be tuned to the Fermi level by strain and a significant anomalous Hall conductivity arises when spin-orbit coupling (SOC) is switched on. A particularly strong SOC effect is identified for X = Ti at $a_{Al2O3} = 4.81$ Å accompanied by an unusually high orbital moment of -0.88 μ_B nearly quenching the spin moment of 1.01 μ_B. The emergence of this orbital magnetism makes the realization of Haldane's model of spinless fermions possible. The extension of this work to the 4d and 5d series led to the identification of cases of high orbital moment (Os) or candidates for Chern insulators (CI), i.e. X = Tc and Pt with C=-2 and -1, depending on the Coulomb repulsion strength. Support by the DFG within CRC/TRR80, project G3 is gratefully acknowledged.

KFM 28.6 Fri 10:45 H 0110

Metal-Insulator Transition in Thin Films and Multilayers of Early Transition Metal Oxides from DFT+DMFT — •Sophie D. Beck and Claude Ederer — Materials Theory, ETH Zürich, Zurich, Switzerland

The wide variety of interesting phenomena and functionalities of complex oxide thin films and heterostructures is generally determined by a number of different factors, such as substrate-induced epitaxial strain, dimensional confinement, interface-related effects, or defects. Here, we systematically study the interplay between these effects in thin films and multilayers composed of materials such as correlated metals, Mott insulators and band insulators, using a combination of density functional theory (DFT) and dynamical mean-field theory (DMFT). In particular, we investigate the evolution of octahedral rotations across interfaces between two materials with different rotation angles and/or tilt systems, and how this affects the range of electronic reconstruction in the interfacial region. We then show that these effecs can give rise to phenomena such as metallic interfaces in multilayers of two Mott insulators $LaVO_3$ and $LaTiO_3$ up to a metal-insulator transition in the correlated metal $CaVO_3$, for which we find that both tensile strain or reduced film thickness can lead to a strong quasiparticle renormalization.

KFM 28.7 Fri 11:00 H 0110

Dimensionality-driven metal-insulator transition in spin-oribt coupled $SrIrO_3$ — •Philipp Schütz[1], Domenico Di Sante[1], Lenart Dudy[1], Judith Gabel[1], Martin Stübinger[1], Martin Kamp[1], Yingkai Huang[2], Massimo Capone[3], Marius-Adrian Husanu[4], Vladimir Strocov[4], Giorgio Sangiovanni[1], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Germany — [2]Van der Waals - Zeeman Institute, University of Amsterdam, Netherlands — [3]CNR-IOM-Democritos National Simulation Center and International School for Advanced Studies (SISSA), Italy — [4]Swiss Light Source, Paul Scherrer Institut, Switzerland

Upon reduction of the film thickness we observe a metal-insulator transition in epitaxially stabilized, spin-orbit coupled $SrIrO_3$ ultra-thin films. By comparison of the experimental electronic dispersions with density functional theory at various levels of complexity we identify the leading microscopic mechanisms, i.e., a dimensionality-induced re-adjustment of octahedral rotations, magnetism, and electronic correlations. The astonishing resemblance of the band structure in the two-dimensional limit to that of bulk Sr_2IrO_4 opens new avenues to unconventional superconductivity by "clean" electron doping through electric field gating.

15 min. break.

KFM 28.8 Fri 11:30 H 0110

Intrinsic defects effects to the electronic structure of Sr_2IrO_4 probed by scanning tunneling microscopy — •Zhixiang Sun[1], Jose M. Guevara[1], Ekaterina M. Pärschke[1], Steffen Sykora[1], Kaustuv Manna[1,2], Johannes Schoop[1], Andrey Malyuk[1], Sabine Wurmehl[1,3], Jeroen van den Brink[1], Bernd Büchner[1,3], and Christian Hess[1] — [1]IFW-Dresden, 01069 Dresden — [2]MPI-CPfS, 01187 Dresden — [3]Institute for Solid State Physics, TU Dresden

Due to its similarity to cuprates, there is tremendous interest on the possible superconducting ground-state in doped Sr_2IrO_4 (Ir214). Nevertheless, it has been found that doping of Ir214 is difficult. The mechanism of dopant induced insulator to metal transition (IMT) has not been fully clarified. We have carried out low temperature scanning tunneling microscopy/spectroscopy experiments on Ir214 crystals. Several different types of intrinsic defects have been identified and their effects to the local electronic structure have been probed. We noticed that for the apical oxygen site defects, their effects are spatially very localized (< 2 nm). Also on the spectra taken on top of these defects, in gap states with a charge transfer like behavior are observed. With a local defect model we simulated the spectra, which gives good a match with the results. Our results provide important observations on the effects of individual defects on the local electronic properties. This is crucial for further tailoring the electronic structure of Ir214. Furthermore, they can also facilitate the understanding of the general mechanism of IMT in Mott insulators.

KFM 28.9 Fri 11:45 H 0110

Novel insights into the impurity-selective metal-insulator transition of paramagnetic V_2O_3 — •Frank Lechermann[1], Noam Bernstein[2], Igor Mazin[2], and Roser Valenti[3] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstr. 9, D-20355 Hamburg, Germany — [2]Code 6393, Naval Research Laboratory, Washington, DC 20375, USA — [3]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

The phase diagram of V_2O_3 with temperature and concentration of different dopants (e.g. Cr and Ti), still poses a formidable problem in condensed matter physics. By means of the charge self-consistent combination of density functional theory with dynamical mean-field theory, i.e. the DFT+DMFT approach, we provide new clues to the delicate interplay between electronic and lattice degrees of freedom. The impact of the defect chemistry is highlighted beyond the sole lattice expansion/contraction affect usually associated with impurity doping in this system. Local symmetry breakings are identified as one key feature to understand the tight competition between metal and insulator in vanadium sesquioxide.

KFM 28.10 Fri 12:00 H 0110

Growth and characterization of *Pmnb*-Li_2FeSiO_4 single crystals — •Waldemar Hergett[1], Christoph Neef[1], Hubert Wadepohl[2], Hans-Peter Meyer[3], Mahmoud Abdel-Hafiez[4], and Rüdiger Klingeler[1,5] — [1]Kirchhoff Institute of Physics, Heidelberg University, Heidelberg, Germany — [2]Institute of Inorganic Chemistry, Heidelberg University, Heidelberg, Germany — [3]Institute of Earth Sciences, Heidelberg University, Heidelberg, Germany — [4]Institute of Physics, Goethe University, Frankfurt, Germany — [5]Center for Advanced Materials, Heidelberg University, Heidelberg, Germany.

Li_2FeSiO_4 single crystals featuring the high temperature *Pmnb* phase were grown by the high-pressure optical floating zone method. The resulting single crystals have been characterized by means of polarised-light and electron microscopy, EDX, powder and single crystal X-ray diffraction. The impact of the growth parameters and of the applied pressure on the crystal quality was investigated. The single crystal structure of the *Pmnb*-polymorph was solved for the first time. It exhibits layers of corner-sharing FeO_4- and SiO_4-tetrahedra in the crystallographic *ac*-planes which alternate with layers of LiO_4-tetrahedra. Magnetisation and specific heat studies confirm the high quality of the crystals and show a sharp λ-like anomaly associated with the onset of long-range antiferromagnetic order at $T_N = 17\,K$.

KFM 28.11 Fri 12:15 H 0110

Excitonic dispersion of intermediate-spin state in $LaCoO_3$ revealed by resonant inelastic X-ray scattering — •Atsushi Hariki[1], Ru-Pan Wang[2], Andrii Sotnikov[1], Federica Frati[2], Jun Okamoto[3], Hsiao-Yu Huang[3], Amol Singh[3], Di-Jing Huang[3], Keisuke Tomiyasu[4], Chao-Hung Du[5], Frenk M. F de Groot[1], and Jan Kuneš[2] — [1]Institute for Solid State Physics, TU Wien, Austria — [2]Inorganic Chemistry and Catalysis, Debye Institute for Nanomaterials Science, Utrecht University, Utrecht, The Netherlands — [3]Condensed Matter Physics Group, National Synchrotron Radiatiation Research Center, Taiwan, — [4]Department of Physics, Tohoku University, Sendai, Japan — [5]Department of Physics, Tamkang University, New Taipei City, Taiwan,

We perform Co *L*-edge resonant inelastic X-ray scattering of $LaCoO_3$ at 20 K. We observe a dispersive state with an energy shift from 480 to 290 meV as a function of momentum from $\boldsymbol{q} = (0, 0, 0.26\pi)$ to $\boldsymbol{q} = (0, 0, 0.90\pi)$. This dispersion is attributed to the mobility of the intermediate-spin (IS) state, which is viewed as an exciton. A theoretical calculation considering the excitonic dispersion of the IS state on the background of the low-spin (LS) state supports the interpretation. The present result suggests that the mobility pushes the IS state into play to the thermal spin-state transition of $LaCoO_3$ in addition to the (immobile) high-spin and LS states with lower atomic-multiplet energies, as suggested by recent theoretical studies [1].

[1] A. Sotnikov and J. Kuneš, Sci. Rep. 6, 30510 (2016).

KFM 28.12 Fri 12:30 H 0110

Electronic signature of the vacancy ordering in NbO (Nb_3O_3) — Anna K. Efimenko[1], Nils Hollmann[1], Katharina Hoefer[1], Jonas Weinen[1], Daisuke Takegami[1], Klaus K. Wolff[1], Simone G. Altendorf[1], Zhiwei Hu[1], A. Diana Rata[1], Alexander C. Komarek[1], Agustinus Nugroho[2], Yen-Fa Liao[3], Ku-Ding Tsuei[3], H. H. Hsieh[4], H. -J. Lin[3], C. T. Chen[3], Liu Hao Tjeng[1], and •Deepa Kasinathan[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Insitiut Teknologi Bandung, Bandung, Indonesia — [3]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [4]Chung Cheng Institute of Technology, Taoyuan, Taiwan

We investigated the electronic structure of the vacancy-ordered 4d-transition metal monoxide NbO (Nb_3O_3) using angle-integrated soft- and hard-x-ray photoelectron spectroscopies as well as ultra-violet angle resolved photoelectron spectroscopy. We found that density-functional-based band structure calculations can describe the spectral features accurately provided that self-interaction effects are taken into account. In the angle-resolved spectra we were able to identify the so-called vacancy band that characterizes the ordering of the vacancies. This together with the band structure results indicates the important role of the very large inter-Nb-4d hybridization for the formation of the ordered vacancies and the high thermal stability of the ordered structure of niobium monoxide.

KFM 28.13 Fri 12:45 H 0110

Ultrahigh-resolution Resonant Inelastic X-ray Scattering from rare-earth nickelates: magnetic and dd-excitations — •Katrin Fürsich[1], Yi Lu[1], Davide Betto[2], Georg Christiani[1], Giniyat Khaliullin[1], Maurits W. Haverkort[3], Eva Benckiser[1],

Matteo Minola[1], and Bernhard Keimer[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart — [2]European Synchrotron Radiation Facility, Grenoble — [3]Institut für Theoretische Physik, Universität Heidelberg

Rare-earth nickelates ($RNiO_3$) have been subject to intense investigation, mostly because of the rich phase diagram comprising a sharp temperature-driven metal-to-insulator transition, an unusual antiferromagnetic ground state, and the prospect of mimicking the physics of high-T_c superconducting cuprates in orbitally engineered heterostructures. We have studied $RNiO_3$ thin-films and superlattices using ultrahigh-resolution resonant inelastic x-ray scattering (RIXS) at the Ni L_3 edge. Below the magnetic ordering temperature, we observe well-defined collective magnon excitations. Our experimental observation provides for the first time a solid basis for the theoretical description of the magnetism in $RNiO_3$. In addition to magnetic excitations, we investigated the electronic excitations of $RNiO_3$ as a function of temperature and tolerance factor, i.e. rare-earth radius. A sophisticated analysis based on an advanced double-cluster model gives intriguing insight into the microscopic and electronic structure of $RNiO_3$. Our study reveals that RIXS is an excellent technique to quantitatively characterize different ordering phenomena within one material.