Dielectric Solids Division
Fachverband Dielektrische Festkörper (DF)

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Overview of Invited Talks and Sessions

(lecture rooms EB 107 and EB 407; Poster E)

Invited and Topical Talks

DF 1.1	Mon	9:30–10:00	EB 107	**Conducting 180° domain walls in PZT thin films** — •Patrycja Paruch
DF 1.2	Mon	10:00–10:30	EB 107	**Charged Domain Walls and Their Impact on Properties of Ferroelectrics** — •Alexander Tagantsev
DF 1.3	Mon	10:30–10:50	EB 107	**UV-induced domain wall conductivity in Lithium Niobate single crystals** — Mathias Schröder, •Alexander Haussmann, Lukas M. Eng
DF 1.4	Mon	10:55–11:25	EB 107	**Mechanisms and control of conduction through domain walls in $BiFeO_3$ thin films** — •Saeedeh Farokhipoor, Beatriz Noheda
DF 1.5	Mon	11:25–11:55	EB 107	**Domain wall functionality in complex oxides** — •Jan Seidel
DF 1.6	Mon	11:55–12:15	EB 107	**Photoinduced electrical transport properties of LiNbO3 single crystals** — •Andreas Thiessen, Alexander Haussmann, Mathias Schröder, Theo Woike, Lukas M. Eng
DF 15.1	Thu	9:30–10:10	EB 107	**Dielectric perovskite oxides: Always good for a surprise** — •Annette Bussmann-Holder
DF 17.1	Thu	15:00–15:30	EB 107	**Wind energy - Characterization and modeling of short-term fluctuations in incoming wind and power output** — •Michael Hölling, Matthias Wächter, Allan Morales, Patrick Milan, Joachim Peinke
DF 17.2	Thu	15:30–16:00	EB 107	**Fluktuationen in der Stromerzeugung aus erneuerbarer Energien: Ihre Charakterisierung und Möglichkeiten ihrer Kompensation** — •Detlev Heinemann
DF 17.3	Thu	16:00–16:30	EB 107	**Glasses and glass ceramics as dielectrics for high power capacitors.** — •Martin Letz
DF 17.6	Thu	17:10–17:40	EB 107	**High Tc Superconducting Energy Storage Systems** — •Frank Werfel
DF 17.7	Thu	17:40–18:10	EB 107	**The transmission of high-power microwaves via dielectric diamond windows: Design, qualification and first steps towards a broadband diamond window in the range of 30GHz to several THz for actual and future fusion devices** — •Theo Scherer, Dirk Strauss

Invited talks of the joint symposium SYXD

See SYXD for the full program of the symposium.

SYXD 1.1	Mon	15:00–15:30	H 0105	**Disputed discovery: The beginnings of X-ray diffraction in crystals** — •Michael Eckert
SYXD 1.2	Mon	15:30–16:00	H 0105	**Why are quasicrystals quasiperiodic?** — •Walter Steurer
SYXD 1.3	Mon	16:00–16:30	H 0105	**Coherent Diffraction Imaging with Free-Eletron Lasers** — •Massimo Altarelli
SYXD 1.4	Mon	16:30–17:00	H 0105	**X-ray free-electron lasers - emerging opportunities for structural biology** — •Ilme Schlichting
SYXD 1.5	Mon	17:00–17:30	H 0105	**Structure analysis by x-ray diffraction and x-ray imaging: beyond crystals, beyond averages, and beyond modeling** — •Tim Salditt

Invited talks of the joint symposium SYRS

See SYRS for the full program of the symposium.

SYRS 1.1	Thu	15:00–15:30	H 0105	**Redox-based resistive memories - recent progress** — •Rainer Waser
SYRS 1.2	Thu	15:30–16:00	H 0105	**Electric Formation of Metal/$SrTiO_3$ Junctions and its Correlation to Multi-Dimensional Defects** — •Dirk C. Meyer, Hartmut Stöcker, Juliane Hanzig, Florian Hanzig, Matthias Zschornak, Barbara Abendroth, Sibylle Gemming
SYRS 1.3	Thu	16:00–16:30	H 0105	**The Connecting between the Properties of Memristive Material Systems and Application Requirements** — •Thomas Mikolajick, Stefan Slesazeck, Hannes Mehne
SYRS 1.4	Thu	16:30–17:00	H 0105	**Mechanism of resistive switching in bipolar transition metal oxides** — •Marcelo Rozenberg
SYRS 1.5	Thu	17:00–17:30	H 0105	**Resistive switching memories: Mechanisms, modeling and scaling** — •Daniele Ielmini

Sessions

DF 1.1–1.6	Mon	9:30–12:15	EB 107	**Focus Session: Conductive Domain Walls**
DF 2.1–2.11	Mon	9:30–12:45	EB 301	**Multiferroics I (jointly with MA, DS, KR, TT)**
DF 3.1–3.3	Mon	15:00–16:00	EB 107	**Nonlinear dielectrics, phase transitions, relaxors**
DF 4.1–4.12	Mon	15:00–18:30	EB 301	**Multiferroics II (jointly with MA, DS, KR, TT)**
DF 5.1–5.2	Mon	16:05–16:45	EB 107	**Electrical, mechanical and electromechanical properties**
DF 6.1–6.3	Mon	16:50–17:50	EB 107	**Application of dielectric solids**
DF 7.1–7.11	Tue	9:30–12:45	EMH 225	**100 years since the Laue experiment: Topical aspects of diffraction and scattering (Joint Session KR, BP, CPP, DF, GP, MA, MI, MM; related to SYXD)**
DF 8.1–8.12	Tue	9:30–12:45	EB 301	**Multiferroics III (jointly with MA, DS, KR, TT)**
DF 9.1–9.90	Tue	12:15–15:15	Poster A	**Poster I - Biomagnetism, FePt Nanoparticles, Magnetic Particles/Clusters, Magnetic Materials, Magnetic Semiconductors, Half-metals/Oxides, Multiferroics, Topological Insulators, Spin structures/Phase transitions, Electron theory/Computational micromagnetics, Magnetic coupling phenomena/Exchange bias, Spin-dependent transport, Spin injection/spin currents, Magnetization/Demagnetization dynamics, Magnetic measurement techniques**
DF 10.1–10.6	Wed	9:30–11:30	EB 407	**High- and low-k-dielectrics (jointly with DS)**
DF 11.1–11.8	Wed	9:30–12:20	EB 107	**Optical and nonlinear optical properties, photonic**
DF 12.1–12.1	Wed	12:25–12:45	EB 107	**Nano- and microstructured dielectrics**
DF 13.1–13.28	Wed	15:00–17:30	Poster E	**Poster II**
DF 14.1–14.4	Wed	15:00–17:30	Poster E	**Poster III – 100 years since the Laue experiment: Topical aspects of diffraction and scattering (Joint Session KR, BP, CPP, DF, GP, MA, MI, MM)**
DF 15.1–15.5	Thu	9:30–11:35	EB 107	**Dielectric and ferroelectric thin films**
DF 16.1–16.2	Thu	11:40–12:20	EB 107	**Dielectric surfaces and interfaces**
DF 17.1–17.7	Thu	15:00–18:10	EB 107	**Focus Session: Alternative energies – Compensation of long- and short-term fluctuations (jointly with DY)**
DF 18.1–18.5	Fri	9:30–10:45	H 0111	**Resistive switching I (jointly with DS, KR, HL)**
DF 19.1–19.6	Fri	11:00–12:30	H 0111	**Resistive switching II (jointly with DS, KR, HL)**

Jahreshauptversammlung des Fachverbandes Dielektrische Festkörper

Mittwoch 18:00–19:00 EB107

- Bericht des Fachverbandleiters
- Analyse des bisherigen Tagungsverlaufes
- Hinweise zur Wahl des Vorstandsrates der DPG
- Ausblick auf die Wahl des DF-Vorstandes 2013
- Verschiedenes

DF 1: Focus Session: Conductive Domain Walls

Organisation: Lukas Eng (Technische Universität Dresden)

Time: Monday 9:30–12:15 Location: EB 107

Invited Talk DF 1.1 Mon 9:30 EB 107

Conducting 180° domain walls in PZT thin films — •Patrycja Paruch — DPMC, University of Geneva, Geneva, Switzerland

Following the recent discovery of conduction at ferroelectric domain walls in otherwise insulating BiFeO3 thin films, we have investigated Pb(Zr0.2Ti0.8)O3 epitaxial thin films using atomic force microscopy (AFM) techniques to identify new functional properties. 180° domain walls in this material show not only a piezoelectric shear response forbidden by symmetry in the bulk material, but also present a current signal in conductive tip AFM. The observed domain wall conduction is clearly differentiable from polarization switching currents, and shows highly nonlinear and asymmetric current-voltage characterisitics, strong temperature dependence at higher temperatures, and high stability. Potential conduction mechanisms will be discussed, specifically in relation to the asymmetric nature of the electrodes contacting the ferroelectric thin film, and the microscopic structure of the domain walls promoting defect segregation.

ref: J. Guyonnet et al, Adv. Mat. 23, 5377 (2011)

Invited Talk DF 1.2 Mon 10:00 EB 107

Charged Domain Walls and Their Impact on Properties of Ferroelectrics — •Alexander Tagantsev — Swiss Federal Institute of Technology

A ferroelectric domain wall can carry net bound charge depending on its orientation with respect to the direction of polarization in adjacent domains. The properties of such walls, called charged walls, can substantially differ from those of walls which carry no bound charge. An essential feature of this kind of walls is that, practically, they can exist only when their bound charge is nearly fully screened by free carriers in the material.

This paper is devoted to the theory of properties (structure, mobility, and conductivity) of charged ferroelectric domain walls and that of the impact of this kind of walls on the dielectric and piezoelectric properties of the material. Available experimental data will be discussed in the context of the theories presented.

Topical Talk DF 1.3 Mon 10:30 EB 107

UV-induced domain wall conductivity in Lithium Niobate single crystals — Mathias Schröder, •Alexander Haussmann, and Lukas M. Eng — Institute of Applied Photophysics, Technische Universität Dresden, D-01062 Dresden, Germany

For the last years, electronic conduction at ferroelectric domain walls (DWs) in thin films has triggered extensive research activities regarding possible nanoelectronic applications [1,2,3]. Here, we show that this effect is not restricted to thin film systems, but can be observed in highly insulating bulk single crystals as well, according to theoretical predictions [4]. In ferroelectric lithium niobate, DW conductivity can be switched and adjusted by super bandgap illumination ($\lambda \leq 310$ nm) within a broad intensity range at room temperature. Furthermore, we demonstrate that this photo-induced DW conductivity can be elegantly tuned by engineering the tilting angle of the DWs with respect to the polar axis. Our experimental results were obtained using conductive atomic force microscopy (c-AFM) under UV illumination to map the DW conductivity with a resolution in the nm range.

[1] J. Seidel et al. *Nat. Mater.* **8**, 229 (2009).
[2] S. Farokhipoor et al. *Phys. Rev. Lett.* **107**, 127601 (2011).
[3] J. Guyonnet et al. *Adv. Mater.* **23**, 5377 (2011).
[4] M. Y. Gureev et al., *Phys. Rev. B* **83**, 184104 (2011).

5 min. break

Invited Talk DF 1.4 Mon 10:55 EB 107

Mechanisms and control of conduction through domain walls in $BiFeO_3$ thin films — •Saeedeh Farokhipoor and Beatriz Noheda — Zernike Institute, Univ. of Groningen, The Netherlands

$BiFeO_3$ (BFO) has become widely popular not only because it is the only room temperature, antiferromagnetic ferroelectric, but also because of the interesting sequence of phase transitions that it can display. In BFO thin films under epitaxial strain different types of domain walls can be obtained with very high control, which has allowed systematic investigation of the distinct properties of domains walls. It was revealed that artificially-written 109^o and 180^o domain walls in BFO thin films show enhanced conductivity with respect to the domains[1]. This promises to enable novel nano-devices and has initiated further work on the mechanisms that control ferroelastic domain wall conductivity in BFO[2,3] and other ferroelectrics[4,5]. Here we show that highly-stable, as-grown, 71^o domain walls of BFO conduct as good as or better than written 109^o walls and that the main mechanism for conduction is thermionic emission of electrons from the top electrode (the conductive tip of an atomic force microscope). The tunability and control of the current by engineering the tip-BFO Schottky barrier using various routes will also be discussed.

[1] J. Seidel et al. Nat. Mat. 8, 229 (2009); [2] J. Seidel et al. Phys. Rev. Lett. 105, 197603 (2010); [3] S. Farokhipoor and B. Noheda Phys. Rev. Lett. 107, 127601 (2011); [4] P. Maksymovych et al. Nanotechn. 22, 254031 (2011); [5] J. Guyonnet et al. Adv. Mater., DOI: 10.1002/adma.201102254

Invited Talk DF 1.5 Mon 11:25 EB 107

Domain wall functionality in complex oxides — •Jan Seidel — Lawrence Berkeley National Laboratory, Berkeley CA 94720, USA

Interfaces and topological boundaries in complex oxide materials, such as domain walls, have recently received increasing attention due to the fact that their properties, which are linked to the inherent order parameters of the material, its structure and symmetry, can be completely different from that of the bulk material. I will present recent results on electronic and optical properties of ferroelectric domain walls in multiferroic BiFeO3 and ErMnO3. The origin and nature of the observed electrical conductivity at certain wall types is probed using a combination of conductive atomic force microscopy, high resolution transmission electron microscopy and first-principles density functional computations.

Topical Talk DF 1.6 Mon 11:55 EB 107

Photoinduced electrical transport properties of LiNbO3 single crystals — •Andreas Thiessen[1], Alexander Haussmann[1], Mathias Schröder[1], Theo Woike[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden — [2]Institute of Structural Physics of Condensed Matte, Technische Universität Dresden, D-01062 Dresden,Germany

Both the photo-induced electronic transport and the photovoltaic properties of domain walls (DWs) have triggered an increased interest in bulk and thin-film ferroic materials [1,2]. Technologically, the electronic behavior of domain walls in bulk LiNbO3 (LNO) single crystals are of special interest due to the availability of large-scale LNO wavers and the possibility of photolithographic domain wall engineering in these materials [3]. In the present work the transport properties of macroscopically contacted LNO were investigated. The temperature and illumination dependence of the electrical conductivity will be discussed, paying particular attention to the microscopic transport mechanisms and activation energies needed for transport within the domain wall regions.

[1] J. Seidel et al., Nat. Mater. 8, 229-234 (2009).
[2] J. Seidel et al., Phys. Rev. Lett. 107, 126805 (2011).
[3] A. Haußmann et al., Nano Lett. 9, 763-768 (2009).

DF 2: Multiferroics I (jointly with MA, DS, KR, TT)

Time: Monday 9:30–12:45 Location: EB 301

Topical Talk DF 2.1 Mon 9:30 EB 301

Reversible electrical switching of spin polarization in multiferroic tunnel junctions — •Marin Alexe, Daniel Pantel, Silvana Götze, and Dietrich Hesse — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle

Spin polarized transport in ferromagnetic tunnel junctions, characterized by tunnel magnetoresistance, has already proven a high application potential in the field of spintronics and in magnetic random access memories (MRAM). Until recently, in such a junction the insulating barrier played only a passive role keeping apart the ferromagnetic electrodes in order to allow electron tunneling. However, a new dimension was added to these devices by replacing the insulator with a ferroelectric material, which possesses permanent dielectric polarization switchable between two stable states. The obtained multiferroic tunnel junction (MFTJ) is a non-volatile memory device with four states, given by two possible ferroelectric polarization directions in the barrier and two different magnetization alignments of the electrodes. Here, we will show that due to the coupling between magnetization and ferroelectric polarization at the interface between a magnetic electrode and the ferroelectric barrier of a MFTJ, the spin polarization of the tunneling electrons can be reversibly and remanently inverted by switching the ferroelectric polarization of the barrier. Selecting the spin direction of the tunneling electrons by short electric pulses in the nanosecond range rather than by an applied magnetic field is highly relevant for spintronics, especially for spin-based information technology.

DF 2.2 Mon 10:00 EB 301

First Principles Modelling of Spin Transport in Functional Oxide Tunnel Junctions — •Nuala M. Caffrey, Thomas Archer, Ivan Rungger, and Stefano Sanvito — School of Physics and CRANN, Trinity College Dublin, Ireland

Spin-dependent tunnelling between ferromagnetic electrodes separated by insulating oxide barriers has long attracted scientific and commercial interest. In the last decade it became evident that the insulating layer was more than just a simple barrier through which electrons tunnel. It is wave-function symmetry selective, making the tunnelling process sensitive to its electronic structure. The understanding of such a concept suggests that one can engineer the transport properties of a tunnel junction by carefully selecting the insulating barrier and the metallic electrodes. Ferroelectric materials are of particular interest as barriers due to additional functionality offered by the electric polarisation.

We investigate, from first-principles, the properties of a multifunctional tunnel junction combining two materials with different ferroic states (ferromagnetic and ferroelectric). We demonstrate massive tunnelling magnetoresistance (TMR) in a SrRuO3 / BaTiO3 / SrRuO3 junction. We also consider the implications of introducing structural asymmetry into this junction by using a thin layer of dielectric material at one interface. In such a junction we demonstrate a sizable tunnelling electroresistance (TER) that increases with the thickness of the dielectric layer.

DF 2.3 Mon 10:15 EB 301

FeO at Iron/Oxide interfaces — •Andrea Neroni, Daniel Wortmann, Ersoy Sasioglu, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We present density-functional theory (DFT) based first-principles calculations of tunneling and magnetoconductance properties of nanoferronic devices consisting of oxide barriers between iron contacts. Several experimental works have indicated the presence of an iron-oxide layer at the contacts of this barrier, that can significantly alter the tunneling properties of the junction. The effect of this layer is still unclear. From the theoretical point of view, one unexplored point are the electron correlations in the single FeO layer at the interface. We account for these correlations with a Hubbard U parameter determined by the constrained random phase approximation (cRPA) [1] and calculate the change of the tunneling magnetoresistance ratio under this condition, using the full-potential linearized augmented plane wave (FLAPW) method `FLEUR` [2]. The electronic transport properties of nanoferronic junctions have been investigated using an embedded Green-function approach [3].

Work is supported by Helmholtz Young Investigators Group Program VH-NG-409 .

[1] E. Şaşıoğlu, C. Friedrich, and S. Blügel, PRB **83**, 121101(R) (2011)
[2] www.flapw.de
[3] D. Wortmann, H. Ishida, and S. Blügel. PRB **66**, 075113 (2002)

DF 2.4 Mon 10:30 EB 301

Thermally stimulated currents in $BiFeO_3$ — •Akash Bhatnagar, Ayan Roy Chaudhuri, Dietrich Hesse, and Marin Alexe — Max Planck Institute of Microstructure Physics, Weinberg 2, Halle(Saale), Germany

Bismuth ferrite($BiFeO_3$)-BFO is a well known multiferroic material, with high ferroelectric Curie temperature (1103 K) and a saturated ferroelectric hysteresis with a remnant polarization of 100 C/cm^2. However, it has been found that pure BFO usually exhibits a high leakage current that could limit wide applications of this material. The thermally stimulated current (TSC) technique was used to get insights into the electronic origin of the leakage, which includes the study of energy levels that might be present in the band gap. These levels can act as trapping centers for charge carriers, thus affecting conductivity. Three systems of BFO, namely, single crystals, thin films and ceramics were studied. Measurements for ceramics and single crystals were performed in capacitor mode, whereas for thin films in-plane electrodes were made using a normal lift-off process. The effect of orientation of the electrodes with respect to domain patterns in thin films, have been investigated. Consequently, trap activation energies and density calculations were performed to fully characterize different levels. Photoconductive and photovoltaic properties were also investigated which corroborate the TSC data.

DF 2.5 Mon 10:45 EB 301

Preparation and characterization of multiferroic thin films grown with an Oxid-MBE — •Paul Zakalek, Markus Waschk, Alexander Weber, and Thomas Brückel — Jülich Centre for Neutron Science JCNS und Peter Grünberg Institut PGI, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

An oxygen-assisted Molecular Beam Epitaxy (MBE) gives the possibility to engine artificial materials on a nanoscale with promising effects. With our machine it is possible to grow complex materials like $La_xSr_{1-x}MnO_3$ (LSMO) or $La_xBi_{1-x}MnO_3$ (LBMO) with remarkably good crystalline quality.

The materials show a variety of interesting effects. For example the La concentration affects the magnetic and electric properties of this systems. The LSMO and LBMO layers can either be antiferromagnetic, ferromagnetic or multiferroic, depending of the La concentration.

Different LSMO/LBMO systems were grown with oxygen-assisted MBE on a $SrTiO_3$ (STO) substrate with different La concentrations. We will present the preparation process and the structural in-house characterization of this systems. First results show good structural quality, like surface roughnesses of not more then one unit cell. Additionally magnetic and electric measurements of the samples will be shown.

15 min. break

DF 2.6 Mon 11:15 EB 301

Guest molecules in ABX3 metal-organic frameworks: multiferroicity and magnetoelectricity — •Alessandro Stroppa[1], Prashant Jain[2], Paolo Barone[1], Martijn Marsman[3], Juan Manuel Perez-Mato[4], Anthony K. Cheetham[5], Harold W. Kroto[2], and Silvia Picozzi[1] — [1]CNR-SPIN, L'Aquila, Italy — [2]Department of Chemistry and Biochemistry, Florida State University Tallahassee, FL 32306 (USA) — [3]University of Vienna, Faculty of Physics and Center for Computational Materials Science (Austria) — [4]Departamento de Fisica de la Materia Condensada Facultad de Ciencia y Tecnologia, UPV/EHU, Bilbao (Spain) — [5]Department of Materials Science and Metallurgy University of Cambridge (UK)

Metal-organic frameworks (MOFs) are increasingly regarded as promising materials. MOFs with perovskite architecture have recently branched out into the field of multiferroics, materials which have both magnetic and ferroelectric orders. Here, we focus on a MOF compound

and theoretically show that it is ferroelectric and this ferroelectricity is the cause of a weak ferromagnetic coupling. In inorganic perovskite-like compounds, octahedral tilting and Jahn-Teller distortions are usually non-polar modes. In this MOF, however, their cooperative link to A-groups via hydrogen bondings finally breaks inversion symmetry, and induces a ferroelectric polarization. We show that the switching of polarization direction implies the reversal of the weak ferromagnetic component, therefore allowing the long-sought electrical control of the magnetization.

DF 2.7 Mon 11:30 EB 301

magnetoelectric effects in the cubic ferrimagnet Cu_2OSeO_3 — •Maria Eleni Belesi[1,2], Mohamed Abid[1], Helmuth Berger[1], and Jean-Philippe Ansermet[1] — [1]Institute of Condensed Matter Physics, EPFL, Station 3, CH-1015 Lausanne, Switzerland — [2]Leibniz Institute for Solid State and Materials Research, Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany

We present magnetic and dielectric measurements in single crystals of the cubic magnetoelectric compound Cu_2OSeO_3. The magnetic measurements show a transition to a ferrimagnetic state at 60 K. This state shows a finite magnetocapacitance which is temperature dependent and varies significantly upon changing the direction of the magnetic field with respect to the crystallographic axes. The magnetocapacitance is also shown to vary with the relative orientation of the magnetic and electric fields. In addition, we found that the magnetically ordered state shows a magnetic field induced electric polarization, whose temperature dependence and anisotropic properties will be discussed.

DF 2.8 Mon 11:45 EB 301

Microscopic Mechanisms for Magnetoelectric Effect in $LiMPO_4$ (M=Mn,Fe,Co,Ni) — •Andrea Scaramucci, Eric Bousquet, and Nicola Spaldin — Materials Theory, Department of Materials, ETH Zurich, Zurich, Switzerland

We theoretically investigate the microscopic mechanisms leading to the linear magnetoelectric effect in the $LiMPO_4$ series. This is of particular interest since some of its constituents possess toroidal moments and shows large magnetoelectric effect.

By using symmetry analysis we obtain the microscopic couplings between spins and electric polarization responsible for each component of the magnetoelectric tensor. Furthermore, we identify couplings with exchange-strictive and relativistic origin. By using *ab initio* calculation and by enforcing numerous non collinear spin configurations we extract the strength of these couplings together with the exchange coupling constants. We use mean field approximation and Monte Carlo simulation to calculate the temperature evolution of magnetoelectric tensor. Our calculations explain the features of the temperature dependence found in experiments.

DF 2.9 Mon 12:00 EB 301

Manipulation of the antiferromagnetic structure in $LiNi_{(1-x)}Fe_xPO_4$ (x = 0.03, 0.2) by iron substitution — •Anne Zimmermann[1] and Manfred Fiebig[1,2] — [1]HISKP, University of Bonn, Germany — [2]Materials Department, ETH Zurich, Switzerland

The LiMPO$_4$ system (M = Fe, Ni, Co, Mn) includes crystallographically isostructural compounds with antiferromagnetic (AFM) order differing in the spin direction only. Thus, the system offers the opportunity to study fundamental mechanisms of AFM 180° domain formation in a range of similar but not identical compounds.

In order to investigate the interplay between the different types of spin order $LiNi_{(1-x)}Fe_xPO_4$ samples with different mixing ratios of nickel and iron were studied using optical second harmonic generation (SHG). SHG coupling linearly to the AFM order parameter was identified in spectroscopy measurements and used for domain imaging. A small iron substitution of $x = 0.03$ yields no change in the domain pattern as well as in the magnetic structure in contrast to pure $LiNiPO_4$. However, for an iron substitution of $x = 0.2$ the spin structure changes significantly: the spin direction lies in the yz-plane and thus between the two spin directions for $LiNiPO_4$ and $LiFePO_4$. The change in magnetic structure is revealed in a different domain pattern as well. Furthermore the order parameter exhibits an unusual, photosensitive temperature dependence which is discussed in detail.

- Work supported by the SFB 608 of the DFG.

DF 2.10 Mon 12:15 EB 301

Multiferroicity and magnetoelectricity in a doped topological ferroelectric — Marco Scarrozza, Maria Barbara Maccioni, Giorgia M. Lopez, Alessio Filippetti, and •Vincenzo Fiorentini — Dept of Physics, U of Cagliari and CNR-IOM, Cagliari, Italy

$La_2Ti_2O_7$ is a "topological" ferroelectric where dipoles are produced by antiferrodistortive rotations failing to compensate due to the layered structure. To turn on multiferroicity, we investigated magnetic doping from first-principles within density-functional theory. The isovalent substitution of Mn for Ti produces antiferromagnetism at all dopings as expected due to superexchange between Mn d^3 ions. In the fully-substituted compound $La_2Mn_2O_7$, many ordering patterns compete, the lowest being a variant of G-type antiferromagnetism. The same system is also magnetoelectric, because the rotations are involved in both magnetic and ferroelectric order: as a coercive field undoes the rotations and depolarizes ferroelectricity, magnetic coupling doubles in intensity. However, the ferromagnetic phase of $La_2Mn_2O_7$ is always much higher in energy. On the other hand, we find that heterovalent substitution of Ti with Cr, Sc, and V always yields robust ferromagnetism. In particular, V orders in rows orthogonal to the P direction, with a covalency gap of 0.2 eV: $La_2Ti_{2-x}V_xO_7$ is therefore properly multiferroic. We are currently investigating the magnetoelectric tensors.

DF 2.11 Mon 12:30 EB 301

***Ab initio* study of the properties of $BaTiO_3$/Co-Pt alloy interface** — •Konstantin Z. Rushchanskii, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut, Forschungszentrum Jülich and JARA,52425 Jülich, Germany

Multiferroics are materials which exhibit more that one ferroic order parameter. They can be made of a single phase, where multiple ferroic order parameters co-exist simultaneously, or of composites, where different ferroic order parameters are combined in separate phases. Due to the limited number of known single phase multiferroics, most of which present multiple ordering only at low temperatures, engineering of composite junctions based on interfaces of magnetic and ferroelectric compounds are therefore of great scientific interest but are also promising due to their potential applications.

Cobalt-platinum alloys are known as compounds with a strong potential for applications in magnetic data storage, due to the strong exchange interactions and strong spin-orbit coupling (and, as a consequence, a large magnetocrystalline anisotropy energy). We present results of *ab initio* calculations based on density functional theory (DFT) of the magneto-electric coupling in cobalt-platinum alloys interfaced with $BaTiO_3$ ferroelectric.

We acknowledge the support by Helmholtz Young Investigators Group Program VH-NG-409.

DF 3: Nonlinear dielectrics, phase transitions, relaxors

Time: Monday 15:00–16:00 Location: EB 107

DF 3.1 Mon 15:00 EB 107

Ferroelectric transition in $LiNbO_3$ calculated from first principles — •Simone Sanna and Wolf Gero Schmidt — Lehrstuhl für Theoretische Physik, Universität Paderborn

Lithium niobate ($LiNbO_3$, LN) belongs to the most important ferroelectric materials. It is furthermore one of the most important optic materials, being the equivalent in the field of non-linear optics and optoelectronics to silicon in electronics [1]. Despite the extensive technological usage, the knowledge of the mechanisms underlying the ferroelectric phase transition is rather poor. The nature of the phase transition itself (displacive or order-disorder) is still argument of debate [2]. In this contribution we report on our first-principles theoretical studies of the ferroelectric transition, which is described in detail at the microscopic level. Total energy calculations as well as long-run molecular dynamics simulations are used to understand the driving forces and mechanisms of the phase transition. Our calculations show that

the structural phase transition is not an abrupt event, but rather a continuous process occurring over about 100 K and involving different ionic species at different temperatures. Because of the different behavior of the Li and Nb sublattice, the ferroelectric transition displays both displacive and order-disorder character. In addition to pure materials, the role of the widely used dopant Ti is investigated, and the results of existing experiments explained in the light of our theoretical models. [1] A. Räuber, Chemistry and Physics of Lithium Niobate (North-Holland Publ. Company, Current Topics in Mat. Sci., 1978). [2] I. Inbar and R. E. Cohen, Phys. Rev. B 53, 1193 (1996).

DF 3.2 Mon 15:20 EB 107

Comparison of hydrostatic and chemical pressure in lead-free $Na_{0.5}Bi_{0.5}TiO_3$-based materials studied by first-principles methods — •Melanie Gröting[1], Silke Hayn[1], Igor Kornev[2], Brahim Dkhil[2], and Karsten Albe[1] — [1]Materialwissenschaft, TU Darmstadt, Darmstadt, Germany — [2]Laboratoire SPMS, Ecole Centrale Paris, Chatenay-Malabry, France

$Na_{0.5}Bi_{0.5}TiO_3$-based materials show extraordinarily high strains and are thus promising environmentally friendly alternatives to the toxic lead-containing standard piezoelectric materials. $Na_{0.5}Bi_{0.5}TiO_3$ is considered as a model relaxor ferroelectric with a complex perovskite structure having two different cations (Na^+ and Bi^{3+}) on the A-site.

In this contribution, the influence of hydrostatic pressure and chemical substitution on ferroelectric instabilities and octahedral tilting in $Na_{0.5}Bi_{0.5}TiO_3$-based solid solutions is studied by first-principles methods. In pure $Na_{0.5}Bi_{0.5}TiO_3$ under positive pressure an orthorhombic Pbnm phase is stabilized above few GPa in good agreement with experimental data. While the polarization is "killed" leaving only tilts under positive pressure, for negative pressure the polarization survives whereas the tilts are suppressed leading to a tetragonal P4mm phase. We find that solid solutions of $Na_{0.5}Bi_{0.5}TiO_3$ with $CaTiO_3$ or $BaTiO_3$ show the same sequence of phase transitions as pure $Na_{0.5}Bi_{0.5}TiO_3$ under hydrostatic pressure and identify the origin of chemical pressure. Chemical substitution leads to a combination of both misfit and modulus effects due to differences in ionic sizes and chemical bonding properties of the different A-cations, respectively.

DF 3.3 Mon 15:40 EB 107

Investigation of the ferroelectric phase transition at silver sodium nitrite using noise measurements — •Jumna Mehlis, Ulrich Straube, and Martin Diestelhorst — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle

The thermal current noise in the vicinity of the ferroelectric-paraelectric phase transition was studied. For this purpose silver sodium nitrite is well-suited, because of its low relaxation frequencies. The current noise density of a short-circuited single crystal was amplified by a low noise operational amplifier. The noise spectra were measured as a function of the temperature by using a spectrum analyzer. The results are in agreement to the Nyquist theorem. That means the noise density is proportional to the temperature and the losses. Contrary to ohmic resistors the thermal noise density of ferroelectrics depends on the frequency. Moreover, the measured spectra show a characteristical change of the shape in dependence on the temperature. This change is strongly correlated with the ferroelectric phase transition temperature, which was determined by the simultaneously measured dielectric function.

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

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

Invited Talk DF 4.1 Mon 15:00 EB 301

Anisotropic conductance of ferroelectric domain walls — •Dennis Meier — Dept. of Physics, University of California, Berkeley, USA

Domain walls are natural interfaces that can exhibit structural, physical, and chemical properties which drastically differ from the surrounding bulk material. This applies to a large variety of phenomena including chemical/electrical transport, multiferroicity, or superconductivity. In addition to the fascinating physical properties domain walls are small in size and their position can be controlled rendering them interesting for future device design. In my talk I report on the exotic nature of trimerization-polarization domain walls in hexagonal $ErMnO_3$. Using piezoforce-response microscopy and conductive atomic force microscopy we revealed that the domain walls represent a structural discontinuity being electrically dressed. While the structural component basically guarantees stability, the electrical dressing generates interesting and new nanoscale physics that I will discuss. The ferroelectric domain walls in $ErMnO_3$ for instance exhibit highly anisotropic electrical properties resulting in directional domain wall conductance. Remarkably, the local electrical conductance is a continuous function of the domain wall orientation which can be explained as a combined consequence of electrostatic and band-structure changes at the walls.

DF 4.2 Mon 15:30 EB 301

Structures and energetics of domain walls in polar hexagonal manganites — •Yu Kumagai and Nicola Spaldin — Department of Materials, ETH Zurich

We use first-principles density functional calculations to study the domain walls in the multiferroic hexagonal manganites, h-$R$$MnO_3$ (R=Sc, Y, Dy–Lu). These materials show an improper ferroelectricity induced by structural trimerization, resulting in $2 \times 3 = 6$ domains (2 for ferroelectricity and 3 for trimerization origin) below the Curie temperature with an intriguing cloverleaf pattern of domains [1,2]. Our calculations explain the observation that ferroelectric (FE) domain walls exist only in combination with antiphase DWs. We find that interlocked ferroelectric and antiphase domain walls have lower energies than typical FE domain walls in conventional ferroelectrics, as well as a much narrower wall width; both factors result from the layered geometry of the h-$R$$MnO_3$ structure.

[1] T. Choi *et al.*, Nature Mater. 9, 253 (2010).
[2] T. Jungk *et al.*, Appl. Phys. Lett. 97, 012904 (2010).

DF 4.3 Mon 15:45 EB 301

Hexagonal $InMnO_3$ - An Outsider Among The Family Of Multiferroic Hexagonal Manganites — •Martin Lilienblum[1], Yu Kumagai[1], Alexei A. Belik[2], Naemi Leo[1], Nicola A. Spaldin[1], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zurich — [2]International Center for Materials Nanoarchitectonics, NIMS

So far, it was believed that hexagonal (h-) $InMnO_3$ exhibit the same type of multiferroic order as the other compounds from the h-$RMnO_3$ family (R = Sc, Y, Dy - Lu), including, in particular, a unit-cell-tripling improper ferroelectric order. Here we present experimental evidence for the *absence* of ferroelectricity in hexagonal $InMnO_3$ based on three different techniques: x-ray diffraction (XRD), piezoresponse force microscopy (PFM) and optical second harmonic generation (SHG). XRD data are ambiguous because they can be described likewise by the non-ferroelectric $P\bar{3}c$ structure and by the ferroelectric $P6_3cm$ structure present in the other h-$RMnO_3$ compounds. However, PFM at room temperature and SHG measurements at low temperature uniquely reveal the absence of ferroelectric order in $InMnO_3$. We therefore propose that $InMnO_3$ exhibits antiferrodistortive, but non-ferroelectric order according to the $P\bar{3}c$ symmetry. Density functional calculations show that the relative energy between the $P\bar{3}c$ and $P6_3cm$ structures is determined by a competition between electrostatic and covalency effects, with an *absence* of covalency favoring the ferroelectric structure. We gratefully acknowledge the support by DFG through SFB 608.

DF 4.4 Mon 16:00 EB 301

Direct observation of multiferroicity in $TbMnO_3$ thinfilms — •Artur Glavic[1], Jörg Voigt[1], Enrico Schierle[2], Eugen Weschke[2], and Thomas Brückel[1] — [1]Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszeutrum Jülich GmbH, Jülich, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, BESSY II, Albert-Einsteinstr. 15, Berlin, Germany

Multiferroic rare earth manganites as $TbMnO_3$ have been studied a lot in the past ten years because of their complex magnetic structure, which leads to a ferroelectric polarization. So far investigations on $TbMnO_3$ thin films grown on $LaAlO_3$ or $SrTiO_3$ showed an emergent

ferromagnetism, destroying the multiferroic properties.

We have investigated $TbMnO_3$ films grown with sputter deposition on $YAlO_3$ substrates using soft x-ray resonant magnetic scattering with linear and circular polarized light. By measuring the circular dichroism originating from the chirality of the magnetic structure we could directly observe multiferroic domains in the thin films. Although the transition temperatures found were comparable to bulk, an additional influence of the Tb magnetic order on the ferroelectricity was observed.

DF 4.5 Mon 16:15 EB 301

Sinusoidal electromagnon in RMnO$_3$: Indication of anomalous magnetoelectric coupling — •Markku Stenberg[1] and Rogério de Sousa[2] — [1]Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany — [2]Department of Physics and Astronomy, University of Victoria, Victoria, B.C., V8W 3P6, Canada

The optical spectra in the family of multiferroic manganites $R\mathrm{MnO}_3$ is a great puzzle. Current models can not explain the fact that two strong electromagnons are present in the non-collinear spin cycloidal phase, with only one electromagnon surviving the transition into the collinear spin sinusoidal phase. We show that this is a signature of the presence of anomalous magnetoelectric coupling that breaks rotational invariance in spin space and generates oscillatory polarization in the ground state.

DF 4.6 Mon 16:30 EB 301

Neutron scattering studies on chiral multiferroics: magnetic structure and excitations — •Max Baum[1], Thomas Finger[1], Jeannis Leist[2], Karin Schmalzl[3], Paul Steffens[3], Petra Becker[4], Ladislav Bohatý[4], Götz Eckold[2], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Physikalische Chemie, Georg-August-Universität Göttingen — [3]Institut Laue Langevin (ILL), Grenoble — [4]Institut für Kristallographie, Universität zu Köln

Multiferroic materials or compounds with a strong magnetoelectric effect posses a large application potential in data storage techniques. Quite recently, systems with a peculiar spiral magnetic order were shown to directly induce a spontaneous electric polarisation and to exhibit giant magnetoelectric effect. Neutron scattering with spherical polarisation analysis gives access to the chiral component of the magnetic structure which is directly linked to the electric polarisation. Therefore, it is possible to control the chiral components by an external electric field. We present neutron scattering experiments on IN14 and IN20 using spherical polarisation analysis documenting the poling of the elastic magnetic chiral terms for MnWO4, TbMnO3 and Ni3V2O8 by cooling in an electric field. In addition, it is possible to switch the chiral components by varying the electric field at constant temperature; thereby measuring multiferroic hysteresis curves. For MnWO4, this experiment was performed with time resolution detecting the typical relaxation times. Tor TbMnO3 we discuss a newly discovered excitation which exhibits a chirality opposite to the static one.

DF 4.7 Mon 16:45 EB 301

Theoretical study of Magnetoelectric effects in Multiferroic RMn2O5 — •Safa Golrokh Bahoosh[1], Julia Wesselinowa[2], and Steffen Trimper[3] — [1]Max Planck Institute of Microstructure Physics, 06099 Halle, Germany — [2]Department of Physics, University of Sofia, 1164 Sofia, Bulgaria — [3]Institute of Physics, Martin-Luther-University, 06120 Halle, Germany

The magnetoelectric behavior of the rare-earth RMn2O5 perovskites is studied theoretically using a quantum model. Whereas the magnetic subsystem is described by nearest-neighbor ferromagnetic coupling and next nearest neighbor antiferromagnetic order, the ferroelectric subsystem is characterized by an Ising model in a transverse field.

Due to frustration, the magnetic system offers spiral structures. The coupling between both systems is a symmetry-allowed linear coupling.

Using Green*s functions we find analytically the temperature and wave vector dependent elementary excitation of the Magnetoelectric system, the polarization and the magnetization for different magnetoelectric coupling strengths.

Lowering the temperature, the system undergoes a magnetic transition at TN and a further reduction of the temperature leads to a ferroelectric transition at TC $<$ TN. The magnetoelectric coupling is manifested as a kink in both the magnetization and the elementary excitation at TC. The polarization is enhanced under the presence of a finite external magnetic field. In the same manner the magnetization is slightly changed by an applied electric field near to TC.

15 min. break

DF 4.8 Mon 17:15 EB 301

Origin of spin canting in multiferroic perovskites — •Carlo Weingart, Eric Bousquet, and Nicola Spaldin — Materials Department, ETH Zurich, Switzerland

In magnetic perovskites with oxygen octahedral distortions, it is usually admitted that the Dzyaloshinsky-Moriya interaction (DM) is responsible for the spin canting. This statement is however partially true since the single-ion anisotropy (SIA) can also allow for similar spin canting. By decomposing the different magnetic interactions (exchange, DM and SIA) from first-principles calculations, we show that depending on the magnetic cation, the DM and the SIA can be of similar amplitude. This allow us to reconsider the origin of the weak ferromagnetism in multiferroics.

DF 4.9 Mon 17:30 EB 301

A further step of understanding the complex magnetic order in magnetoelectric Co_3TeO_6 — •Vera Carolus[1], Thomas Lottermoser[2], Matthias Hudl[3], Pierre Tolédano[4], and Manfred Fiebig[2] — [1]HISKP, University of Bonn, Germany — [2]Department of materials, ETH Zurich, Switzerland — [3]Department of Engineering Sciences, Uppsala University, Box 534, SE-751 21 Uppsala, Sweden — [4]Laboratory of Physics of Complex Systems, University of Picardie, 33 rue Saint-Leu, 80000 Amiens, France

Like most of the known magnetoelectric multiferroics, Co_3TeO_6 exhibits a complex spin structure with a series of consecutive phase transitions. Contrary to common compounds, Co_3TeO_6 possesses two independent commensurate k-vectors in the multiferroic low-temperature phase. In addition, magnetic-field dependent measurements of the ferroelectric polarization show a strongly anisotropic behaviour.

Here we show our results using spatially resolved optical second harmonic generation (SHG) under external magnetic and electric fields in the multiferroic low-temperature phase. However, the SHG gives only access to the magnetic subsystem. Like the ferroelectric polarization, the magnetic structure shows strongly anisotropic behaviour. In crossed magnetic and electric fields we were able to reach a single-domain state, while a magnetic field solely always leads to distinctively different multi-domain states. Most remarkably, for a certain direction of magnetic field, we were able to invert the multi-domain state. Furthermore, this behaviour indicates the existence of a pronounced memory effect.

DF 4.10 Mon 17:45 EB 301

The multiferroic, geometric frustrated $CuCrO_2$ compound: a case of the $p-d$ hybridization spin-charge coupling? — •Matthias Frontzek, Georg Ehlers, and Andrey Podlesnyak — Neutron Scattering Science Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

Multiferroic materials have become of interest for their unusual low-temperature properties in general, and in particular for the observation that one can affect their magnetic structure through an electric field and their electric polarization through a magnetic field. The delafossite $CuCrO_2$, which crystallizes in the rhombohedral $R\bar{3}m$ space group, is a multiferroic compound with an apparent strong coupling of spin and charge. In contrast to other multiferroic compounds $CuCrO_2$ shows a spontaneous electric polarization upon antiferromagnetic ordering without an accompanying structural phase transition, although a slight in-plane lattice distortion has been measured.

In our contribution, we present a detailed study on $CuCrO_2$ single crystals using neutron diffraction and spectroscopy as well as pulsed magnetic field measurements up to 60 T of the electric polarization. Based on our study we will show a revised magnetic structure model and present a model Hamiltonian including in-plane next-next nearest neighbor and inter-layer exchange interaction. We will stress the importance of the latter for the multiferroic properties and will show evidence based on the high field polarization measurements that the proposed $p-d$ hybridization spin-charge coupling mechanism needs to be modified.

DF 4.11 Mon 18:00 EB 301

Theory of High-Temperature Multiferroicity in CuO — •Naëmi Leo[1,2], Pierre Tolédano[3], Dmitry D. Khalyavin[4], and Manfred Fiebig[1,2] — [1]ETH Zurich, Switzerland — [2]HISKP, Universität Bonn, Germany — [3]University of Picardie, France — [4]ISIS, United Kingdom

Spin-spiral multiferroics offer strong magnetoelectric coupling, although most of them have low transition temperatures which make them undesirable for technical applications. Cupric oxide is a remarkable exception with its high Curie temperature of 230 K. Understanding the interactions leading to such a high-T_C magnetically induced ferroelectricity is very desirable for future room-temperature magnetoelectric multiferroics devices.

Here we present a Landau theory analysis of the multiferroic properties of CuO [1]. Using a multi-dimensional order parameter expansion of the free energy we examine the sequence of phase transitions: The unusual direct transition to the multiferroic phase is induced by the simultaneous onset of two order parameters, enabled by the strong Cu-O superexchange. Expressing the order parameter in terms of spins we determine theoretically the magnetic structure in the spin-spiral phases. Furthermore we identify the microscopic interactions responsible for the magnetically induced spontaneous polarization.

The work in Bonn was supported by the DFG through the SFB 608.

[1] P. Toledano, N. Leo, D.D. Khalyavin, L.C. Chapon, T. Hoffmann, D. Meier, and M. Fiebig, Phys. Rev. Lett. **106**, 257601 (2011).

DF 4.12 Mon 18:15 EB 301

Resonant Elastic X-ray Scattering Studies of Multiferroic $NdFe_3(BO_3)_4$ — •Sven Partzsch[1], Jorge Enrique Hamann-Borrero[1], Claudio Mazzoli[2], A. Vasiliev[3], L. Bezmaternikh[4], Bernd Büchner[1], and Jochen Geck[1] — [1]IFW, Dresden, Germany — [2]ESRF, Grenoble, France — [3]Moscow State University, Moscow, Russia — [4]L. V. Kirensky Institute of Physics, Russian Academy of Sciences, Krasnoyarsk, Russia

Multiferroic $NdFe_3(BO_3)_4$ exhibits a strong magnetoelectric coupling, since at 2K the electric polarization raises rapidly to 400 μC/m^2 upon increasing the applied magnetic field to 2T [1]. We study this coupling by resonant x-ray scattering at the Nd L- and Fe K edges as a function of temperature and applied magnetic field. Employing full polarization control, the field dependence of the different magnetic phases has been characterized at the Nd L_2 edge. We find that the commensurate phase at 20K and no magnetic field is different from the commensurate phase induced by the magnetic field at 2K [2].

[1] A. Zvezdin et al., JMMM, 300, 224 (2006)
[2] J. E. Hamann-Borrero et al., Phys. Rev. B, 82, 094411 (2010)

DF 5: Electrical, mechanical and electromechanical properties

Time: Monday 16:05–16:45 Location: EB 107

DF 5.1 Mon 16:05 EB 107

Calibrated real time detection of nonlinearly propagating giant strain waves — •André Bojahr[1], Marc Herzog[1], Daniel Schick[1], and Matias Bargheer[1,2] — [1]Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Wilhelm-Conrad-Röntgen Campus, BESSY II, Albert-Einstein-Str. 15, 12489 Berlin, Germany

Epitaxially grown metallic oxide films excited by femtosecond laser pulses can generate giant strain amplitudes on the order of 1% strain. We calibrate these transient strain amplitudes by ultrafast X-ray diffraction (UXRD). In addition we use picosecond reflectivity measurements to determine the speed of the propagating strain fronts by interference effects which are equivalent to stimulated Brillouin scattering [1]. For high strain amplitudes we observe two components of the sound pulses which travel at different sound speeds. We conclude that at giant strain amplitudes the compressive and tensile strain components travel at different sound velocities [2]. This is indicative of an anharmonic interaction between the atoms forming the crystal lattice which give rise to nonlinearities in the wave equation.

[1] Thomsen *et al.*, Phys. Rev. B 34, 4129 (1986)
[2] P. J. S. van Capel and J. I. Dijkhuis, Appl. Phys. Lett 88, 151,910 (2006).

DF 5.2 Mon 16:25 EB 107

Piezoelectric properties of single ceramic fibres: Comparison of two methods — •Sabine Kern, Christoph Pientschke, and Ulrich Straube — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle

Composites containing piezoelectric fibres embedded in a polymer matrix are used for sensoric, actuatoric and ultrasonic applications. Accurate knowledge of the piezoelectric properties of the fibres is desirable to optimise these materials. In this work, the determination of the small-signal piezoelectric coefficient d_{33} of ceramic PZT-fibres was realised with two methods by using a capacitive displacement sensor. On the one hand, the effective d_{33} of 1-3 fibre composites is measured. Then the d_{33} of the fibres can be calculated using the ceramic's and polymer's elastic properties and the fibre volume content. Independently, the d_{33} of the fibres was determined directly by measuring the longitudinal piezoelectric strain. PZT-fibres with 250 μm in diameter and 1-3 composites with a fibre volume content ν of 35% and 65% that contain these fibres were studied. The measurements at single fibres show well-reproducible values with a small standard deviation for the d_{33}, whereas the local measurements at composites show a larger range of variation in their effective d_{33}, especially for composites with lower ν. This higher variance is mainly influenced by the locally highly varying fibre volume content and less by the fibre properties themselves. Moreover, composites with larger ν show higher d_{33} than composites with lower ν. Finally, the d_{33} of single fibres derived from the composites' properties was compared with the directly measured values.

DF 6: Application of dielectric solids

Time: Monday 16:50–17:50 Location: EB 107

DF 6.1 Mon 16:50 EB 107

Dielectric pore-free glass-ceramic materials with good metal adhesion properties for GHz applications — •Hubertus Braun[1,2], Martin Letz[2], and Martun Hovhannisyan[2] — [1]Johannes Gutenberg-Universität Mainz — [2]Schott AG, Mainz

In recent years, the continuous growth in mobile communication technologies operating in the microwave frequency range demands cost-efficient low-loss dielectric materials with sufficiently high relative permittivity. Conventional microwave devices like antennas or filter elements which operate close to lossy materials, such as human tissue, decrease their performance due to additional dielectric losses (*Body Loading* effects). These effects can be prevented by using *Dielectric Loading*. Therefore metallised low-loss high permittivity ceramics ($\varepsilon_r \approx$ 20-80) are needed which allow a high concentration of the EM near-field inside the dielectric and thereby a reduction of external influences. An additional advantage of dielectric loaded devices lies in their smaller size compared to conventional pure metal devices, following the miniaturisation trend of microelectronics of the last decades.

A possible alternative to conventional sinter-ceramic fabrication techniques is glass-ceramic technology in which the desired geometries can be cast to net shape followed by crystallisation to achieve intrinsic pore free materials with the desired dielectric properties and comparatively superior metal adhesion properties. In the current work, promising glass-ceramics in the Rare-Earth-Titanate system are analysed concerning suitability for DLA applications and comparative measurements are made with commercially used sinter-ceramics.

DF 6.2 Mon 17:10 EB 107

Time dependent properties of ferroelectric electron emission from PMN-PT single crystals — •Jana Becherer, Oliver Mieth, and Lukas M. Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

We report on the electron emission properties of PMN-PT single crystals upon cyclic switching using a variety of different voltage shapes. An aperture in the top electrode allows electrons to exit from the ferroelectric solid into vacuum. The emission current was measured under

UHV conditions using a single electron detector. We find that the emitted electron current strongly depends on both the duty cycle and repetition rate of the applied voltages. Comparative measurements of the polarization switching in the samples were performed. The polarization switching occurs over a broad distribution of time as is typical for relaxor PMN-PT. We found that the electron emission is strongly correlated with the amount of reversed polarization.

DF 6.3 Mon 17:30 EB 107

Voltage tunable polymer laser device — •Matthias Kollosche[1], Sebastian Döring[2], Joachim Stumpe[2], and Guggi Kofod[1] — [1]ACMP, Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany — [2]Fraunhofer Institute for Applied Polymer Research, PPC, Geiselbergstr. 69, Potsdam-Golm, 14476, Germany

Organic laser materials offer a broad optical gain spectra they are predestined for the realization of tunable laser sources. Here we report on a compact organic laser device that allows for voltage controlled continuous wavelength tuning in the visible range of the spectrum without the usage of an external motion control. The compact optical element consists of an elastomeric distributed feedback (DFB) laser and an electro active elastomer actuator also known as artificial muscle. To enable direct wavelength tuning the elastomer laser is placed in the centre of the prepared actuator. The chosen configuration geometry and electrode distribution of the elastomeric actuator gives rise to homogeneous compression in the centre of the actuator. The voltage induced deformation of the artificial muscle is transferred to the elastomeric laser and results in a decrease of grating period. This leads to an emission wavelength shift of the elastomer laser. The increase of actuation voltage to 3.25 kV decreased the emission wavelength of the laser device from 604 nm to 557 nm, a change of 47 nm or 7.8%.

DF 7: 100 years since the Laue experiment: Topical aspects of diffraction and scattering (Joint Session KR, BP, CPP, DF, GP, MA, MI, MM; related to SYXD)

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

Invited Talk DF 7.1 Tue 9:30 EMH 225

The discovery of X-ray interferences, the role of characteristic radiation therein and potential applications of the Laue method in modern engineering. — •Hans-Jürgen Ullrich[1], Siegfried Däbritz[2], Enrico Langer[2], Jürgen Bauch[1], Andreas Danilewsky[3], and Peter Paufler[4] — [1]Institute of Materials Science at the TU Dresden — [2]Institute for Solid State Physics at the TU Dresden — [3]Institute of Crystallography at the University of Freiberg — [4]Institute of Structural Physics at the TU Dresden

It was during a noteworthy conversation between Paul Peter Ewald and Max von Laue in the English Garden in Munich in early 1912 that the foundation for the discovery of X-ray interferences was laid. They were debating which effects can be expected when short-wave electromagnetic radiation is allowed to impinge on crystals, and in a eureka moment Max von Laue theorized that interference phenomena are caused.

The first diffraction experiments were founded on the notion that the interferences in question might be characteristic radiation. The effect subsequently searched for was eventually discovered by Walther Kossel and his colleagues in 1934 (interferences from lattice sources, Kossel interferences). It is with this fact in mind that our lecture will look at the significance of Laue and Kossel diffraction patterns during the initial research into X-ray physics and their influence on all further academic work in this area. In the past, Laue's discovery was mainly applied within the natural sciences, but more recently the Laue method has also been employed successfully in engineering, for example:

- for quality assessment procedures used within the framework of semiconductor chip production
- as diagnostic techniques for gas turbine blades.

DF 7.2 Tue 10:00 EMH 225

Thermal diffuse scattering as a complementary tool in the study of lattice dynamics — Björn Wehinger, Alexeï Bosak, and •Michael Krisch — ESRF, 6 Rue Jules Horowitz, BP 220, 38043 Grenoble, France

Thermal diffuse scattering (TDS) in combination with inelastic x-ray scattering (IXS) and lattice dynamics calculations allows the reconstruction of the lattice dynamics in the entire Brillouin zone. X-ray scattering by thermally populated phonons in crystals reduces the intensity of Bragg spots and substantially increases the intensity of the diffuse scattering which has a rich structure in reciprocal space [1,2]. In combination the two techniques can serve as a rigorous benchmark for parameter free lattice dynamics calculations [3]. The proposed method can be used for the precise detection of mode softening, for the study of lattice dynamics under extreme conditions and for time resolved measurements. In metallic systems it is possible to map the Fermi surface in tree dimensions by directional tracing of Kohn anomalies [4]. The presented results on β-tin illustrate the functionality of the proposed combined approach with new insights into the dynamical properties on this system.

[1] Wooster, Diffuse X-ray reflections from crystals, Clarendon Press, Oxford (1962)
[2] Xu RQ, Chiang TC, Z. Kristallogr. 220, 1009 (2005)
[3] A. Bosak, et al., Z. Kristallogr. preprint: doi: 10.1524/zkri.2012.1432
[4] A. Bosak, et al., PRL, 103, 076403 (2009)

DF 7.3 Tue 10:15 EMH 225

Brillouin scattering of ultrashort optical and x-ray pulses from quasi-monochromatic phonon wavepackets — •Marc Herzog[1], André Bojahr[1], Jevgenij Goldshteyn[2], Steffen Mitscherling[1], Wolfram Leitenberger[1], Dmitry Khakhulin[3], Michael Wulff[3], Ionela Vrejoiu[4], Roman Shayduk[2], Peter Gaal[1], and Matias Bargheer[1,2] — [1]Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [3]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [4]European Synchrotron Radiation Facility, Grenoble, France

We excite a $SrRuO_3$ thin film transducer epitaxially grown on a $SrTiO_3$ substrate with pulse trains of ultrashort laser pulses. Each laser pulse launches single bipolar strain pulses of broad bandwidth into the substrate [1] which coherently add up to form a quasi-monochromatic sub-THz phonon wavepacket. The generation and dynamics of these phonon pulses is investigated by Brillouin scattering using visible and hard x-ray photons. The combination of both methods reveals the excited narrow phonon spectrum as well as the phonon lifetime which is on the order of a few 100 ps in the considered frequency range. This lifetime is explained by anharmonic phonon interactions.

[1] Thomsen *et al.*, Phys. Rev. B 34, 4129 (1986).

DF 7.4 Tue 10:30 EMH 225

Following Strain-Induced Mosaicity Changes of $PbZr_{0.2}Ti_{0.8}O_3$ Thin Films by Ultrafast Reciprocal Space Mapping — •Daniel Schick, André Bojahr, Marc Herzog, Peter Gaal, and Matias Bargheer — Institut für Physik & Astronomie, Universität Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam/Golm

We studied the propagation of coherent sound waves in a $PbZr_{0.2}Ti_{0.8}O_3$ (PZT) - $SrRuO_3$ (SRO) bilayer sample after optical excitation of the metallic SRO layer. We observed changes of the out-of-plane lattice constant and structure factor of the ferroelectric PZT layer that can be exclusively attributed to the transient strain wave launched from within the SRO layer. In addition to this we are also able to follow in-plane structural dynamics simultaneously utilizing a new ultrafast reciprocal space mapping technique. Thereby we observed a transient change of the mosaicity of the PZT layer on a ps timescale which is again directly coupled to the coherent sound wave travelling through the layer.

DF 7.5 Tue 10:45 EMH 225

Analysis of the size and shape of colloidally prepared nanocrystals by Rietveld refinement — •Holger Borchert, Xiaodong Wang, Marta Kruszynska, Joanna Kolny-Olesiak, and

Jürgen Parisi — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, Carl-von-Ossietzky Str. 9-11, 26129 Oldenburg, Germany

Many properties of colloidal nanocrystals can be tuned by controlling the crystal size and shape. Examples are the quantum size effect in the case of semiconductors or size-dependent catalytic properties in the case of metals. Establishing correlations between the structure and other properties relevant for applications requires suitable methods to characterize the size and shape of nanocrystals. Most evident are imaging techniques like transmission electron microscopy (TEM). However, as a disadvantage only a limited number of particles can be evaluated. Powder X-ray diffraction (XRD), in contrast, probes a large ensemble of nanocrystals, but it remains a challenge to reliably extract information on the crystallite size and shape from XRD data. In this work, colloidal chemistry was used to prepare mono- and bimetallic Pt and Pt/Sn nanocrystals as well as semiconductor nanocrystals of ZnO, CuInS2 and composite particles consisting of CuInS2 and Cu2S. The samples were analyzed by TEM and XRD. Rietveld refinement of XRD data was done with a program enabling to simulate also anisotropic crystallite shapes. This approach turned out to be suitable for the determination of the average size and shape, in particular also in the case of nanorods and composite nanomaterials.

DF 7.6 Tue 11:00 EMH 225

Strain measurement in semiconductor nanostructures by convergent electron nanoprobe diffraction — •Knut Müller[1], Andreas Rosenauer[1], Marco Schowalter[1], Josef Zweck[2], Rafael Fritz[3], and Kerstin Volz[3] — [1]Universität Bremen, Germany — [2]Universität Regensburg, Germany — [3]Universität Marburg, Germany

The fundamental but simple Bragg law is exploited to measure lattice strain with a precision of $7 \cdot 10^{-4}$ and a spatial resolution of $0.5-0.7$ nm directly from convergent beam electron diffraction (CBED) patterns. In particular, we present 3 different algorithms for pattern recognition to measure CBED reflection positions accurately: The first detects edges in a patch around each CBED disc and iteratively finds all edge points which lie on the disc boundary by circle fitting. The second takes a rotational average in the patch and maximises the gradient in radial direction by optimising the centre of the rotational average. The third and fastest method exploits cross-correlations between each reflection patch and different types of masks. Besides results for a 350 nm wide $In_xGa_{1-x}N_yAs_{1-y}$/GaAs highly strained quantum layer stack with alternating compressive/tensile strain, we present prospects for the operation and acquisition hardware of a TEM, directly deduced from the three algorithms above to allow for a fast strain map acquisition directly at the microscope in future. For the present study we operated an FEI Titan (S)TEM microscope in STEM mode to record a series of energy filtered CBED patterns on CCD.

15 min. break

DF 7.7 Tue 11:30 EMH 225

Theory of Electron Magnetic Circular Dichroism — •Jan Rusz — Dept. of Physics and Astronomy, Uppsala University, Sweden

Electron magnetic circular dichroism (EMCD) is an electron microscopy analogue of the established x-ray magnetic circular dichroism, that can provide atom-specific spin and orbital moments. EMCD, compared to its x-ray counterpart, offers a potential of significantly better spatial resolution, potentially in the Angstrom range. Presently, the technique is limited by difficulties of reaching sufficient signal to noise ratio and complexity of the accompanying dynamical diffraction effects, both of which make quantitative analysis demanding and prone to systematic errors.

We present recent theoretical developments in the field of EMCD, namely, 1) influence of plural scattering and associated spectral post-processing corrections; 2) convergence of the dynamical diffraction calculations in electron energy loss spectroscopy (ELNES), and 3) decomposition of the signal in diffraction plane to maps of various irreducible operators, such as orbital and spin magnetic moments, number of holes, orbital and spin-orbital anisotropy tensors.

These developments improve our understanding of deviations of recent quantitative EMCD experiments from expected values, allow more accurate predictions of the signal distribution, and uncover the wealth of information contained in electron energy loss spectra and thus aid in improving the methods of extraction of the magnetic signal from experimental datasets.

DF 7.8 Tue 11:45 EMH 225

Magnetic structure of magnetoelectric $NdFe_3(BO_3)_4$ under applied magnetic fields — •Jorge E. Hamann-Borrero[1], Sven Partzsch[1], Sergio Valencia[2], Claudio Mazzoli[3], Christian Hess[1], A. Vasiliev[4], L. Bezmaternikh[5], Bernd Büchner[1], and Jochen Geck[1] — [1]IFW-Dresden — [2]Helmholtz-Zentrum-Berlin — [3]ESRF, Grenoble, France — [4]Moscow State University, Russia — [5]L. V. Kirensky Institute of Physics, Russian Academy of Sciences, Krasnoyarsk, Russia

The magnetic structure of the magneto-electric $NdFe_3(BO_3)_4$ is studied by means of Resonant X-ray Magnetic Scattering (RXS) at the Nd $L_{2,3}$ and Fe K edges. The temperature dependent experiments show below $T_N = 30$ K the appearance of commensurate (CM) magnetic superlattice reflections with Miller indices $(0, 0, l \pm 3/2)$ (where $l = 3n$ and n = integer). By further cooling, at $T_{ICM} \sim 16$ K, a transition into an incommensurate (ICM) spin helix structure is observed in agreement with recent neutron experiments[1, 2]. Detailed mean field based analysis of the x-ray diffracted intensities show, that the Nd and Fe magnetic sublattices behave differently. In fact the magnetization of the Nd sublattice is induced by the Fe moments. At $T<T_{ICM}$, by applying an external magnetic field **B** parallel to the *ab*-plane, the magnetic structure suffers a reorientation transition from a spin helix configuration to a collinear structure where all the moments align perpendicular to **B** in the basal plane.

[1] M. Janoschek et al. Phys. Rev. B, 2010, 81, 094429
[2] P. Fischer et al. Jour. Phys. Cond. Matt., 2006, 18, 7975-7989(15)

DF 7.9 Tue 12:00 EMH 225

Monoclinic Symmetry in Barium Titanate — Christian Eisenschmidt, •Hans Theo Langhammer, and Günther Schmidt — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik

The tetragonal-orthorhombic phase transition of barium titanate crystals has been investigated by XRD measurements during slow cooling. Additional diffuse scattering intensity between the (002) and (200) reflexes as well as a shift of the (200) reflex towards higher 2Θ values develop with decreasing temperature and time. The tetragonal-orthorhombic phase transition takes place obviously via a monoclinic intermediate stage. This can be understood by assuming this order-disorder phase transition is initiated by increasing short-range order (SRO) of Ti ions followed by rearranging of Ba ions similar to the 'tetragonal' SRO below the Burns temperature above the transition cubic-tetragonal. This results, finally, in nucleation and transition to the long-range ordered orthorhombic phase. Conclusions of the proposed mechanism in compositionally disordered systems like Ba(Ti,Sn)O3, PMN-PT et al. are discussed.

DF 7.10 Tue 12:15 EMH 225

Multilayer Optics for Modern X-ray Analytical Equipment — •Andreas Kleine, Jörg Wiesmann, Bernd Hasse, Jürgen Graf, Uwe Heidorn, Steffen Kroth, Frank Hertlein, and Carsten Michaelsen — Incoatec GmbH, Max-Planck-Str. 2, 21502 Geesthacht, Germany

Even 100 years after the first publication of the Bragg equation, there are current developments which are still mainly based on this fundamental law. One of these developments are multilayer optics which are used for beam shaping of X-rays e.g. for focusing the X-rays onto the sample. The multilayer optics simulate an artificial crystal with the typical distance d of the Bragg equation. It is advantageous that this distance can be changed and thus adapted to the specific application and setup. The development of multilayer optics allowed a performance increase of modern diffractometers by more than one order of magnitude.

In this contribution, we will give an overview of current developments of multilayer optics. We will explain the design and the manufacturing process of the optics and give some examples of typical applications which benefit from the new possibilities, especially in combination with modern microfocus X-ray sources. Applications like GISAXS, high-pressure XRD or micro-diffraction known from synchrotrons, can be realized now in the home-lab.

DF 7.11 Tue 12:30 EMH 225

Reconstruction phenomena at the interfaces of $LaCoO_3$ single films: A resonant x-ray reflectivity study — •Jorge E. Hamann-Borrero[1,2], Abdullah Radi[2], Woo Seok Choi[3], Sebastian Macke[4], Ronny Sutarto[5], Feizhou He[5], George A. Sawatzky[2], Ho Nyung Lee[3], and Vladimir Hinkov[4] — [1]IFW-Dresden — [2]University of British Columbia, Vancouver, Canada —

[3]Oak Ridge National Laboratory, Materials Science and Technology Division, USA. — [4]Max Planck-UBC Centre for Quantum Materials, Vancouver, Canada — [5]Canadian Light Source, Saskatoon, Canada

A series of $LaCoO_3$ (LCO) single films grown on polar $NdGaO_3$ (NGO) and non polar $SrTiO_3$ (STO) substrates were studied by means of Resonant Soft X-ray Reflectivity (RXRR) and X-ray Absorption Spectroscopy (XAS). The RXRR measurements were performed at photon energies close to the Co $L_{2,3}$ edges. The detailed analysis of the energy dependent measurements at fixed Q values corresponding to maxima and minima of the RXRR Kiessig fringes reveals a strong signal contribution to the line-shapes which can not be attributed to pure Co^{3+}. By considering the polar nature of the LCO structure we find that, at interfaces with polar discontinuity, e.g., at LCO/STO and LCO/Vaccum, reconstruction phenomena take place.

The work at Oak Rigde National Laboratory was supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.

DF 8: Multiferroics III (jointly with MA, DS, KR, TT)

Time: Tuesday 9:30–12:45 Location: EB 301

DF 8.1 Tue 9:30 EB 301

Substrate influence on the strain in epitaxially grown $BiCrO_3$ thin films investigated using Raman spectroscopy and X-ray diffraction — •Andreas Talkenberger[1], Cameliu Himcinschi[1], Kannan Vijayanandhini[2], David Rafaja[3], Ionela Vrejoiu[2], Torsten Weissbach[1], Christian Röder[1], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09596 Freiberg — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle — [3]TU Bergakademie Freiberg, Institute of Materials Science, D-09596 Freiberg

$BiCrO_3$ (BCO) is an interesting candidate for multiferroic applications. Therefore a deep understanding of the material properties and the fabrication of high quality epitaxial thin films is necessary. In this work we investigated epitaxially grown BCO thin films fabricated by pulsed laser deposition on $SrTiO_3$, LSAT, $NdGaO_3$ and $DyScO_3$ by means of Raman spectroscopy and X-ray diffraction (XRD). The shift of phonon modes at room temperature indicates different strains in the BCO films grown on the different substrates. Primarily, the XRD experiments helped to quantify the elastic lattice strains caused by the lattice misfit between the substrate and the thin films. The reciprocal space mapping was employed to follow the relaxation of the lattice strain through the formation of microstructure defects. This data was correlated to the observed Raman shifts. Using density functional theory the shifts of the Raman peaks were calculated for different strain states, and compared to the experimentally observed ones. This work is supported by the German Research Foundation DFG HI 1534/1-1.

DF 8.2 Tue 9:45 EB 301

Directly probing the effect of strain on magnetic exchange interactions — •Kathrin Dörr[1,2], Andreas Herklotz[2], Hans-Martin Christen[3], and Michael Biegalski[3] — [1]MLU Halle Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle — [2]IFW Dresden, Postfach 270116, 01171 Dresden — [3]CNMS, Oak Ridge National Laboratory, Oak Ridge, TN 37830, USA

Thin films of transition metal oxides of the perovskite type ABO_3 (B = 3d or 4d metal) have revealed abundant examples for strain-driven changes of magnetic ordering. In spite of strong efforts, the theoretical treatment of magnetic exchange in complex oxides has remained a challenge, and experiments continue to show unpredicted large effects of the epitaxial strains in films. In order to provide meaningful experimental data on strain dependences, epitaxial thin films should be grown in various coherent strain states on different substrates without changing anything but the strain. This is inherently difficult: possible problems arise from a strain-dependent oxidation level or microstructure. As a complementary approach, the in-plane strain of epitaxial oxide films can be controlled reversibly by 0.1-0.2 percent using a piezoelectric substrate. I will address reversible-strain studies on $La_{0.7}Sr_{0.3}MnO_3$, $La_{1-x}Sr_xCoO_3$ (x = 0, 0.2, 0.3) und $SrRuO_3$ films, showing the strain response of the magnetic Curie temperature and the magnetization and discussing the current understanding of the strain effects on magnetic ordering.

DF 8.3 Tue 10:00 EB 301

Induced magnetoelectric response in Pnma perovskites — •Eric Bousquet and Nicola Spaldin — Materials Department, ETH Zurich, Switzerland

We use symmetry analysis to show that the *G*, *C* and *A*-type antiferromagnetic *Pnma* perovskites can exhibit magnetoelectric (ME) responses when a ferroelectric instability is induced with epitaxial strain. Using first-principles calculations we compute the values of the allowed ME response in strained $CaMnO_3$ as a model system. Our results show that large linear and non-linear ME responses are present and can diverge when close to the ferroelectric phase transition. By decomposing the electronic and ionic contributions, we explore the detailed mechanism of the ME response.

DF 8.4 Tue 10:15 EB 301

Search for strain-induced ferroelectricity in EuO films — •Carsten Becher[1], Masakazu Matsubara[1], Andreas Schmehl[2], Jochen Mannhart[3], Darrell G. Schlom[4], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zürich, Switzerland — [2]Institut für Physik, Universität Augsburg, Germany — [3]Max Planck Institute for Solid State Research, Germany — [4]Department of Materials Science and Engineering, Cornell University, USA

Ferromagnetic EuO arouses a lot of interest due to a multitude of extreme properties, such as an insulator-metal transition, a colossal-exceptional magnetoresistance effect, and nearly 100 % spin polarization of the conduction electrons in the ferromagnetic state. In addition, recent theories predict that EuO becomes ferroelectric under epitaxial strains $\geq$ 4.2 %, suggesting a route to novel multiferroics combining ferromagnetic and ferroelectric order. Here, we use optical second harmonic generation (SHG) to detect changes of the electric as well as magnetic order of EuO thin films. In search of a strain-induced spontaneous polarization, we vary the sample temperature, apply electric and magnetic fields in various configurations, and use different photon energies of the incident laser pulses. So far, we verified that samples strained below 4 % do not display ferroelectricity. However, a new sample batch allows us to present results from EuO films with tensile strains up to 7 %.

DF 8.5 Tue 10:30 EB 301

On the lattice engineering of magnetoelectric couplin — •Michael Fechner and Nicola Spaldin — ETH Zurich, Department for Material Theory,CH-8093 Zurich, Switzerland

We present results of first-principles calculations of the microscopic origin of the linear magnetoelectric (ME) effect in Cr_2O_3. In general such magnetoelectric responses – that is the electric polarization created by an applied magnetic field – are small. Since they are composed of both electronic- and lattice-mediated contributions, however, an increase in the response can in principle be achieved by phonon engineering. Here we investigate this possibility by first calculating how the magnetic interaction parameters are affected by phonon modes of different symmetry, focussing particularly on those that are active in the ME coupling. We find that the exchange interactions are most strongly modified in the non-IR active rotational phonon modes which do not contribute to the ME response. We then calculate the effect on the ME response if these phonons are disabled. Based on our results we suggest new routes for engineering materials with enhanced ME couplings.

DF 8.6 Tue 10:45 EB 301

First principles study of Mn_2O_3 under pressure: Competition between Jahn-Teller distortion and charge disproportionation — •Carmen Quiroga and Rossitza Pentcheva — Dept. of Earth and Environmental Sciences, University of Munich

Contrary to most sesquioxides, which naturally occur in the corundum structure, Mn_2O_3 has a complex crystal structure corresponding to an orthorhombically distorted bixbyite [1], associated with the presence of the Jahn-Teller active Mn^{3+} cation. It has been suggested that the Jahn-Teller effect is inhibited under pressure, which could induce a

phase transition to the corundum structure [2], from where the general transformation sequence of sesquioxides to perovskite and post-perovskite should follow. So far, however, only the post-perovskite has been reported experimentally above 27 GPa [3].

Using density functional theory calculations including an on-site Coulomb repulsion term, we explore the stability of the ambient phase α-Mn_2O_3 (*Pbca*) and candidate high-pressure polymorphs: corundum ($R\bar{3}c$), perovskite phases of Rh_2O_3 II (*Pbcn*) and $GdFeO_3$ (*Pbnm*) type and post-perovskite (*Cmcm*). In particular we focus on the effect of pressure on the charge, spin and structural degrees of freedom. Parallels to the pressure induced phase transitions in $MnTiO_3$ are discussed.

Funding by DFG SPP1236 (PE883/8-1) is acknowledged.

[1] S. Geller. Acta Crystallogr. **B27**, 821 (1971).
[2] C.T. Prewitt et al. Inorg. Chem. **8**, 1985 (1969).
[3] J. Santillán et al. Geophys. Res. Lett. **33**, L15307 (2006).

DF 8.7 Tue 11:00 EB 301

Investigation of Magnetoelectric Coupling in Self Assembled Ferromagnetic/Ferroelectric Heterostructures — •Fikret Yildiz[1], Chan-Ho Yang[2], Sinan Kazan[1], Yoon-He Jeong[2], and Bekir Aktas[1] — [1]Gebze Institute of Technology, Department of Physics, 41400 Gebze-Kocaeli, Turkey — [2]Pohang University of Science and Technology, Department of Physics, Pohang, 790-784 S. Korea

Creating ferromagnetic/ferroelectric heterostructures is a way for developing multifunctional materials which is called multiferroics. Exchange bias may be used to couple a normal ferromagnet to a ferroelectric antiferromagnet and thus create a multiferroic system with nonzero magnetization. In implementing this idea we developed a synthesis method for composite films of MnFe2O4 embedded in BiFeO3 [1]. The method utilizes the Bi volatility to obtain the composite films via thermal annealing of multilayer composed of BiFeO3 and BiMnO3. SEM measurements showed that the cluster size varies depending on the film thickness. The composite films possess both ferroelectric and ferromagnetic properties [1]. Magnetoelectric coupling (MEC) was investigated by Ferromagnetic resonance (FMR) technique. Analysis of FMR data showed that resonance field can be controlled by GHz range electric fields.

[1] C.H. Yang, F. Yildiz, S.H. Lee, Y.H. Jeong, U. Chon, T.Y. Koo, Apply Phys. Lett. 90, 163116 (2007).

DF 8.8 Tue 11:15 EB 301

Strain Determination in Magnetoelectric Composite Systems by X-ray Diffraction Methods — •Christian Koops[1], Madjid Abes[1], Stjepan Hrkac[1], Bridget Murphy[1], Olaf Magnussen[1], Eric Woltermann[2], Henry Greve[2], and Eckhard Quandt[2] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany — [2]Institut für Materialwissenschaft, Christian-Albrechts-Universität zu Kiel, Germany

Understanding the coupling at the interface between magnetostrictive and piezoelectric components in magnetoelectric composites (ME) is essential for the optimization of these composites for sensor applications. A large ME response is only possible if the lattice deformation induced by an external magnetic field in the magnetostrictive material can be transferred efficiently to the piezoelectric material. To study this coupling at the burried interface of ME composites we measured the lattice deformation in ZnO as the piezoelectric component by grazing incidence X-ray diffraction in an external magnetic field, using the high-resolution and high intensity X-ray beam provided by the Diamond Light Source (I16) and PETRA III (P08). We employ samples with thin layers of different magnetostrictive materials, $(Fe_{90}Co_{10})_{78}Si_{12}B_{10}$ and Terfenol-D, on the (001) surface of high quality, single crystalline ZnO substrates. From the Bragg peak positions we determined the interplanar spacings in the ZnO substrates close to the interface and the corresponding strain as a function of the applied magnetic field.

15 min. break

DF 8.9 Tue 11:45 EB 301

Relaxor ferroelectricity in pure and doped magnetite — •Eugen Ruff[1], Florian Schrettle[1], Stephan Krohns[1], Peter Lunkenheimer[1], Victor A. M. Brabers[2], and Alois Loidl[1] — [1]Experimental Physics V, University of Augsburg, 86135 Augsburg, Germany — [2]Department of Physics, Eindhoven University of Technology, 5600 MB Eindhoven, Netherlands

A possible example for a multiferroic material is the extensively studied magnetite Fe_3O_4, which shows charge-order (CO) below the Verwey transition at $T_V \approx 120\,K$ and is ferrimagnetically ordered below $500\,K$[1]. As shown in the present contribution, dielectric spectroscopy reveals a relaxation below T_V, indicating relaxorlike polar order in Fe_3O_4[2]. We find long-range ferroelectric order to be impeded by the continuous freezing of polar degrees of freedom and the formation of a tunneling-dominated glasslike state of electrons at low temperatures. To reveal the origin of the ferroelectric state, whose dielectric signature is partly superimposed by a so called Maxwell-Wagner (MW) relaxation, we have investigated doped samples with Al, Ga, and Mg. The dielectric spectra of these doped samples ($< 2\%$) provide further evidence for the relaxor ferroelectric state of Fe_3O_4 and demonstrate the influence of the MW relaxation.

[1]D. I. Khomskii, J. Magn. Magn. Mater. **306**, 1 (2006).
[2]F. Schrettle *et al.*, Phys. Rev. B **83**, 195109 (2011).

DF 8.10 Tue 12:00 EB 301

Full-potential DFT+U study of orbitally ordered systems: the importance of non-spherical contributions and double counting — •Adam Jakobsson[1,2], Biplab Sanyal[1], Ivetta Slipukhina[2], Marjana Ležaic[2], Ersoy Sasioglu[2], Gustav Bihlmayer[2], and Stefan Blügel[2] — [1]Department of Physics and Astronomy, Uppsala University, 75120 Uppsala, Sweden — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

DFT+U has for many years been a standard method to calculate properties of strongly correlated systems. Initially the method [1] was implemented in DFT-codes using the atomic sphere approximation (ASA) but was later also implemented into full potential DFT-codes. Various flavours of the double counting corrections used in the DFT+U method further add to the variety of different DFT+U functionals. The double counting corrections originally derived in the context of ASA are now routinely applied in full potential codes. Using the FLEUR code [2], we have investigated the importance of the non-spherical potential and the issue of double counting for orbital ordering and magnetism, i.e. properties that play a crucial role in many multiferroic materials. A recent implementation [3] of the constrained-RPA method was used to obtain parameters for the DFT+U calculations. This work was supported by the Young Investigators Group Program of the Helmholtz Association, Germany, contract VH-NG-409.

[1] V. I. Anisimov et al. PRB **44**, 943-954 (1991) [2] www.flapw.de [3] E. Şaşıoğlu et al. PRB **83**, 121101(R) (2011).

DF 8.11 Tue 12:15 EB 301

Ab initio **calculations of the magnetic properties of ordered perovskites** — •Igor Maznichenko[1], Alberto Marmodoro[2], Martin Lüders[3], Zdzislawa Szotek[3], Walter Temmerman[3], Ingrid Mertig[1,2], and Arthur Ernst[2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale), Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle (Saale), Germany — [3]Daresbury Laboratory, Daresbury, Warrington WA4 4AD, Cheshire, United Kingdom

Perovskites are of particular interest in condensed matter physics due to their remarkable electronic and magnetic properties. Colossal magnetoresistance, ferroelectricity, multiferroicity, superconductivity, charge ordering, orbital ordering, metal-insulator transition, Jahn-Teller, and other effects are observed in perovskites. All these properties are strongly depending on the type of cations. Here we present a first-principles study of electronic and magnetic properties of $La_{2/3}Sr_{1/3}MnO_3$ (LSMO), which is a strongly correlated 3*d* transition metal oxide with a Curie temperature of 370 K. For varying La/Sr ratios different types of antiferromagnetism are observed. Using a self-consistent KKR Green function method, we show how the electronic and magnetic properties of LSMO depend on the valency of Mn, ordering of different cations in the lattice, and their relative orientation to each other. The influence of the Mn–O–Mn angle on the double-exchange coupling was examined.

DF 8.12 Tue 12:30 EB 301

Crystal growth and scattering investigations of $YFe_2O_{4-\delta}$ — •Thomas Müller[1], Joost de Groot[1], Jörg Strempfer[2], and Manuel Angst[1] — [1]Peter Grünberg Institut PGI and Jülich Centre for Neutron Science JCNS, JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Deutsches Elektronen-Synchrotron DESY, D-22607 Hamburg, Germany

$LuFe_2O_4$ is attracting attention as proposed multiferroic compound,

but there is much less known about other isostructural rare-earth ferrites. We have grown single-crystals of $YFe_2O_{4-\delta}$ in a CO/CO_2-atmosphere to tune δ. Optimized crystals exhibit a magnetic behaviour identical to highly stoichiometric powder samples, i.e. two hysteretic phase transitions at 228 K and 180 K upon cooling.

Corresponding to these phases single-crystal x-ray-diffraction shows 3D-charge-ordered states, partially not compatible with the phases observed by electron diffraction [1]. At least one additional transition below 160 K, not present in magnetisation, is found in x-ray-diffraction. On one sample we found reflections at ($\frac{1}{3}$, $\frac{1}{3}$,half-integer) at 10 K , identical to the superstructure reflections of $LuFe_2O_4$. Nevertheless sample differences, due to different δ, have to be reviewed.

We further searched for anisotropy by resonant x-ray diffraction and full polarization analysis on superstructure reflections at PETRA III-P09. As for $LuFe_2O_4$ no anisotropy is observed. Although YFe_2O_4 has the same structure as $LuFe_2O_4$, the phases between 100 K and 230 K are totally different, showing much more complex incommensurate ordering. [1] N. Ikeda et al. Ferroelectrics **272**, 309 (2002)

DF 9: Poster I - Biomagnetism, FePt Nanoparticles, Magnetic Particles/Clusters, Magnetic Materials, Magnetic Semiconductors, Half-metals/Oxides, Multiferroics, Topological Insulators, Spin structures/Phase transitions, Electron theory/Computational micromagnetics, Magnetic coupling phenomena/Exchange bias, Spin-dependent transport, Spin injection/spin currents, Magnetization/Demagnetization dynamics, Magnetic measurement techniques

Time: Tuesday 12:15–15:15 Location: Poster A

DF 9.1 Tue 12:15 Poster A

Spin-resolved photoemission spectroscopy of $[\mathbf{Mn_6^{III}Cr^{III}}]^{3+}$ single-molecule magnets (SMM) deposited on surfaces and of Mn compounds as reference substances, cross comparison with XMCD — •Andreas Helmstedt[1], Aaron Gryzia[1], Niklas Dohmeier[1], Norbert Müller[1], Armin Brechling[1], Marc Sacher[1], Ulrich Heinzmann[1], Veronika Hoeke[2], Erich Krickemeyer[2], Thorsten Glaser[2], Mikhail Fonin[3], Samuel Bouvron[3], Philipp Leicht[3], Thomas Tietze[4], and Manfred Neumann[5] — [1]Faculty of Physics, Bielefeld University — [2]Faculty of Chemistry, Bielefeld University — [3]Department of Physics, University of Konstanz — [4]Max-Planck-Institut für Intelligente Systeme, Stuttgart — [5]Department of Physics, University of Osnabrueck

The properties of the Mn-based single-molecule magnet $[\mathbf{Mn_6^{III}Cr^{III}}]^{3+}$ deposited on surfaces are studied. This molecule exhibits a large spin ground state of S_T=21/2 and contains six Mn centres in two bowl-shaped Mn_3-triplesalen units linked by a hexacyanochromate. A preparation method for large-scale homogeneous samples needed for sample scanning to avoid radiation damage will be presented. The spin polarization of Auger electrons emitted from the manganese centres in $[\mathbf{Mn_6^{III}Cr^{III}}]^{3+}$ SMM after excitation with circularly polarized synchrotron radiation has been measured in the paramagnetic phase at selected excitation energies in the Mn-$L_{2,3}$ region. These results will be compared to XMCD data obtained at approx. 2K and 7T. Spin polarization data from Mn_2O_3 and Mn(II)acetate references after excitation at the Mn-$L_{2,3}$ edge are presented as well.

DF 9.2 Tue 12:15 Poster A

High-field ESR and magnetization of a Mn(III)-based single chain magnet — •Y. Krupskaya[1], Z. Tomkowicz[2], M. Rams[2], M. Balanda[3], S. Foro[4], Y. Skourski[5], J. Wosnitza[5], S.K. Nayak[6], J.V. Yakhmi[7], W. Haase[6], V. Kataev[1], and B. Büchner[1] — [1]IFW Dresden, Dresden, Germany — [2]Institute of Physics, Jagiellonian University, Kraków, Poland — [3]H. Niewodniczański Institute of Nuclear Physics PAN, Kraków, Poland — [4]Clemens-Schöpf-Institut für Organische Chemie und Biochemie, Technische Universität Darmstadt, Darmstadt, Germany — [5]Dresden High Magnetic Field Laboratory, Rossendorf, Germany — [6]Eduard-Zintl Institut für Anorganische und Physikalische Chemie, Technische Universität Darmstadt, Darmstadt, Germany — [7]Technical Physics and Prototype Engineering Division, Bhabha Atomic Research Centre, Mumbai, India

We present high-field magnetic study of a Mn(III)-based molecular chain. The compound shows a ferromagnetic hysteretic behavior of the magnetization at relatively high temperatures (up to 3 K). High-field/high-frequency ESR measurements were performed at the excitation frequencies between 332 and 528 GHz in magnetic fields up to 15 T. The frequency dependence of the ESR spectrum yields a g-factor of 1.8 and a negative effective magnetic anisotropy D of around -6.37 K. In addition, pulsed field (up to 60 T) magnetization measurements enabled determination of the effective spin value corresponding to the ground state of the chain. In conclusion, our experimental results indicate the single molecular chain magnet behavior of the studied compound.

DF 9.3 Tue 12:15 Poster A

EPR study of hyperfine interactions in Cu(II)- bis(oxamato) complexes — •A. Aliabadi[1], A. Petr[1], M. A. Abdulmalic[2], T. Rüffer[2], V. Kataev[1], and B. Büchner[1] — [1]IFW Dresden, Dresden, Germany — [2]Institute of Chemistry, Chemnitz University of Technology, Chemnitz, Germany

The hyperfine (HF) coupling of two Cu(II)-bis(oxamato) complexes containing four nitrogen ligands has been investigated using EPR spectroscopy at 10 GHz. The EPR spectra were modeled in order to determine the g-factor and the HF coupling values. First, measurements were performed on a liquid solution at room temperature to obtain isotropic g-factor and HF coupling constants for Cu and N. From the EPR measurements on powder samples we were able to extract the g-tensor and the Cu HF coupling tensor. In addition, the angular dependence of the EPR spectra was studied by rotation of a single crystal in three mutually perpendicular planes. From that the Cu HF coupling tensor was further refined and the N HF coupling tensor was determined. The results indicate that the difference between the determined parameters for two complexes is not significant. However, these parameters are smaller compared to a previous study of Cu(II)-bis(oxamato) complex containing two nitrogen ligands [1]. The results of this work should enable the determination of the spin density distribution between the central metal ion and the ligands in the studied molecules.

[1] B. Bräuer, T. Rüffer, R. Kirmse, J. Griebel, F. Weigend, G. Salvan, Polyhedron. 26 (2007) 1773.

DF 9.4 Tue 12:15 Poster A

Magnetic properties of a mixed valence Ni(II)-Ni(III)-complex as probed by the ESR spectroscopy and static magnetization measurements — •Jaena Park[1,3], Yulia Krupskaya[1], Vladislav Kataev[1], Bernd Büchner[1], Frederik Schleife[2], Berthold Kersting[2], and Rüdiger Klingeler[3] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, Dresden, Germany — [2]Institute of Inorganic Chemistry, University of Leipzig, Leipzig, Germany — [3]Kirchhoff Institute for Physics, University of Heidelberg, Heidelberg, Germany

We investigated magnetic properties of a mixed valence Ni(II)-Ni(III)-complex by means of high-field electron spin resonance spectroscopy and static magnetization measurements. The metal core of the complex contains one Ni^{2+} ion ($S = 1$) and one Ni^{3+} ion ($S = 1/2$) coupled by three sulphur bridges. The magnetic field dependence of the magnetization at low temperatures and the temperature dependence of the static magnetic susceptibility reveal a ferromagnetic coupling between the Ni-spins. The high-field frequency tunable electron spin resonance measurements enable determination of the g-factor and magnetic anisotropy values for the studied complex. In addition, we compare the magnetic properties of the Ni(II)-N(III)-complex with those of the similar structure Ni(II)-N(II)-complex having both Ni ions in the 2+ oxidation state.

DF 9.5 Tue 12:15 Poster A

Electrical characterization of intermetallic FePt nanoparticles — •Ulrich Wiesenhütter[1], Darius Pohl[2], Bernd Rellinghaus[2], Jürgen Fassbender[1], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden Rossendorf, D-01328 — [2]Leibniz-Institut für Festkörper- und

Werkstoffforschung, D-01069

Magnetic nanoparticles have a large potential for applications such as medical diagnosis and therapy, (bio-)sensors or magnetic recording. Conventional techniques, e.g., MFM, electron holography or Lorentz microscopy are only suited to determine magnetical properties of macroscopic particle ensembles. In order to investigate the electrical and magnetic properties of a single, free-standing FePt nanoparticle two nano-sized Au electrodes that are fabricated by electron beam lithography, are used.The full characterization of the particle is carried out by electron microscopy and by recording current-voltage characteristics. As a result Coulomb-blockade effects have been observed at low temperatures. The capacitance of the nanoparticles is derived from the I/V characteristics.

DF 9.6 Tue 12:15 Poster A

Cobalt-Gold Core-Shell Nanoparticles as Probes for Quantitative MFM — •Tino Uhlig[1], Ulf Wiedwald[2], Denny Köhler[1], Paul Ziemann[2], and Lukas Eng[1] — [1]Institut für Angewandte Photophysik, TU Dresden — [2]Institut für Festkörperphysik, Universität Ulm

We present an easy, fast and reliable method for the preparation of magnetic force microscopy (MFM) probes based on single magnetic nanoparticles. Due to their dipole like characteristics, these kind of magnetic probes open up possibilities for quantitative measurements of magnetizations on the nano-scale. Our fabrication method is based on the deposition of cobalt nanoparticles (diameter 30 nm) on a Si substrate and subsequent photochemical deposition of a gold layer on the particle surface. Single particles were attached to standard silicon AFM tips with the aid of a linker molecule (APTMS). The applicability of the fabricated probes was tested by imaging the magnetic domains of a hard disk drive sample. Furthermore a calibration method, using the deflection of the AFM cantilever in an external magnetic field, is presented.

DF 9.7 Tue 12:15 Poster A

Shift of the blocking temperature of Co nanoparticles by Cr capping — •Melanie Ewerlin[1], Derya Demirbas[1], Leonardo Agudo[2], Gunther Eggeler[2], and Oleg Petracic[1] — [1]Institut für Experimentalphysik / Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany — [2]Institute for Materials, Department of Material Science, Ruhr-Universität Bochum, 44780 Bochum, Germany

We have prepared Co nanoparticles (NPs) on Al_2O_3 buffer layers and studied the effect of capping with various amounts of Cr onto the magnetic properties. Structural and magnetometric characterization was performed using TEM and SQUID magnetometry, respectively. The uncapped Co NPs show superparamagnetic behavior with a blocking temperature of T_B=14K. The magnetic properties are strongly influenced by the Cr capping resulting in a decrease of T_B for nominal thicknesses of Cr up to 0.15nm. However, for larger values the blocking temperature increases again. XMCD measurements at the Cr edge indicate an anti-parallel alignment of the magnetic moments in the Cr layer with respect to the moments in the Co particle, which leads to a decrease of the effective magnetic volume and hence to a decrease of T_B. The second regime is governed by inter-particle coupling via Cr-bridges.

DF 9.8 Tue 12:15 Poster A

Interaction effects between self-assembled Co nanoparticles — •Astrid Ebbing[1], Leonardo Agudo[2], Gunther Eggeler[2], and Oleg Petracic[1] — [1]Institut für Experimentalphysik/Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum — [2]Institut für Werkstoffe, Ruhr-Universität Bochum, 44780 Bochum

In this work we present the influence of Pt on self-assembled Co nanoparticles (NPs). We show that capping the Co NPs with Pt results in strong changes in the magnetic properties. With increasing Pt capping we observe a transition from 'demagnetizing' (viz. dipolar) toward 'magnetizing' (e.g. polarization type) interactions between the NPs. We performed magnetization hysteresis, ZFC/FC vs. temperature and delta(M)-measurements using a superconducting quantum interference device magnetometer to investigate the nature of coupling between the NPs. The measurements show negative delta(M)-values for small amounts of Pt capping material and positive values for 0.53 nm Pt or more, which indicates a magnetizing interaction between the NPs via the Pt-bridges.

DF 9.9 Tue 12:15 Poster A

Characterization of superparamagnetic nanoparticles for bone tissue engineering — •M. Uhlarz[1], T. Herrmannsdörfer[1], R. De Santis[2], M. Sandri[3], A. Tampieri[3], E. Figallo[4], T. D'Alessandro[4], S. Keshari-Samal[5], G. Rischitor[6], and the MAGISTER collaboration[7] — [1]Hochfeld-Magnetlabor Dresden, HZ Dresden-Rossendorf — [2]IMCB-CNR, Napoli, Italia — [3]ISTEC-CNR, Faenza, Italia — [4]Fin-Ceramica SpA, Faenza, Italia — [5]ISMN-CNR, Bologna, Italia — [6]Western General Hospital, University of Edinburgh, UK — [7]Europäische Kommission, Bruxelles, Belgique

Currently, large bone or cartilage defects are stabilized by massively-invasive surgery. The permanent implants used for this purpose are either metallic prostheses, or body tissue taken elsewhere from the patient. In a novel tissue-engineering approach, autologous tissue regeneration is guided by implanted magnetic scaffolds under external magnetic field. These scaffolds attract superparamagnetic Fe_3O_4 (magnetite) nanoparticles tagged with Vascular Endothelial Growth Factor (VEGF) molecules. Release of the growth-factor molecules at the scaffold (optionally triggered by ac-field induced hyperthermia) attracts autologous chondrocytes and osteoblasts, which build up fresh bone and cartilage tissue. We report on the magnetic characterization of several biocompatible and biodegradable materials that might serve as scaffold materials.

This project is supported by the European Union's FP7-Cooperation Programme through the MAGISTER project (Magnetic Scaffolds for in-vivo Tissue Engineering), Large Collaborative Project FP7 - 21468.

DF 9.10 Tue 12:15 Poster A

Hall effect in nanodimensional multilayers based on island films of Pd and Fe — •Sergej A. Nepijko[1], Dmytro Kutnyakhov[1], Olena Tkach[2], Larysa Odnodvorets[2], Ivan Protsenko[2], and Gerd Schönhense[1] — [1]Institute of Physics, University of Mainz, 55099, Mainz, Germany — [2]Sumy State University, 40007, Sumy, Ukraine

Nanodimensional n-layers systems of $[Pd/Fe]_n/SiO_2/Si$, where $3 \leq n \leq 10$, were used to examine the Hall effect. Effective thickness of separate layers of Pd and Fe changed in the range from 0.4 to 1.4 nm (Pd) and from 0.6 to 0.9 nm (Fe). Electron microscopic studies indicate that the layers have island structure and their composition corresponds to fcc-Pd and bcc-Fe. Solid solutions of Pd-Fe with fct-lattice are formed only when the thickness of layers $\geq$ 3 nm and after annealing at $\geq$ 790 K. Measurement of Hall coefficient R_H indicate that its value monotonically decreases with increasing number of layers n. For example, for multilayer Pd(1.1 nm)/Fe(0.9 nm) R_H decreases from 5.5×10^{-9} m^3/C (n=2) to 3.97×10^{-9} m^3/C (n=10). A size dependence of R_H is observed also at fixed Fe layer thickness and variable thickness of Pd. For multilayer $[Pd(x)/Fe(0.6)]_{10}$ the Hall coefficient decreases from 4.80×10^{-9} m^3/C to 3.69×10^{-9} m^3/C while increasing the effective thickness of Pd from x= 0.4 to 1.4 nm.

DF 9.11 Tue 12:15 Poster A

Spin-fluctuation energies in 3d transition-metal clusters deposited on Pt (111) — •Sergej Riemer[1], Gustavo Pastor[2], Jesus Dorantes-Dávila[3], and Raul Garibay-Alonso[4] — [1]Universität Kassel, Germany — [2]Universität Kassel, Germany — [3]UASLP, San Luis Potosí, Mexico — [4]Universidad Autónoma de Coahuila, Mexico

A functional-integral theory of itinerant magnetism is applied to transition-metal clusters deposited on Pt (111). The low temperature limit of the local spin-fluctuation energies $\Delta F_l(\xi)$ at different atoms l is determined as a function of the exchange field ξ by using a real-space recursive expansion of the local Green's functions. The size, structural, and local-environment dependence of $\Delta F_l(\xi)$ is calculated for representative examples of Fe_N, Co_N and Ni_N with $N \leq 13$ atoms. The interplay between fluctuations of the module and of the relative orientation of the local magnetic moments is analyzed. Comparison between free and deposited clusters having the same structure and interatomic distances reveals remarkable changes in the spin-excitation spectrum of the clusters as a result of the hybridizations with the metallic support. For instance, in the case of small Fe clusters on Pt (111) one observes that the spin-flip energies are reduced by more than an order of magnitude as a consequence of deposition. A similar important reduction of the Curie temperature is expected. This contrasts with the results for the ground-state magnetic moments and magnetic order, which are essentially the same in the free and deposited configurations.

DF 9.12 Tue 12:15 Poster A

Coupling behavior in iron-oxide nanoparticle/Py thin film composite systems — •Caroline Fink[1], Philipp Szary[1], Giovanni Badini Confalonieri[1], Durgamadhab Mishra[1], Maria Benitez[1,2], Mathias Feyen[2], An-Hui Lu[2], Leonardo Agudo[3], Gunther Eggeler[3], and Oleg Petracic[1] — [1]Institut für Experimentalphysik/Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Max-Planck-Institut für Kohlenforschung, D-45470 Mülheim an der Ruhr, Germany — [3]Institut für Werkstoffe, Ruhr-Universität Bochum, D-44780 Bochum, Germany

We have investigated the magnetic and electrical transport properties of iron-oxide nanoparticle/Py thin film composite systems. Ultrathin films of Permalloy (Py) have been prepared by means of UHV ion beam sputtering and subsequently covered by one monolayer of iron-oxide nanoparticles. Post-annealing of the samples under controlled atmospheric conditions allows us to transform the particles into a mixed wüstite/magnetite (FexO/Fe3O4) phase showing intra-particle exchange bias. A slight variation of the NP type yields systems of different coupling behavior. Performing magnetometry and transport measurements we observe either a strong or weak coupling between the Py film and the NPs depending on the NP type. Moreover, a strongly decoupled behavior can be observed when adding a sapphire (Al2O3) layer separating the particles from the Py. Results have been compared with reference systems consisting of only NPs or only Py.

DF 9.13 Tue 12:15 Poster A

Magnetoresistance properties of Fe_3O_4 nanoparticles in a Cu matrix — •Sergej A. Nepijko[1], Dmytro Kutnyakhov[1], Maxym Demydenko[2], Serhiy Protsenko[2], Dmytro Kostyuk[2], and Gerd Schönhense[1] — [1]Institute of Physics, University of Mainz, 55099, Mainz, Germany — [2]Sumy State University, 40007, Sumy, Ukraine

The aim of the work was the manufacturing of ordered arrays of magnetic Fe_3O_4 nanoparticles, the investigation of their structural and phase state and magneto-resistance in a wide range of annealing temperatures. Nanoparticles were prepared by chemical synthesis and drop deposited onto a Si substrate. After deposition the ordered nanoparticle array was observed by TEM. Nanoparticle sizes changed from 6.0 nm (as deposited) to 11.6 nm (after annealing at 1200 K). The phase state of the nanoparticles was cubic (spinel type) with lattice parameter varying from 0.811 nm (as-deposited) to 0.840 nm (1200 K). The magnetoresistance was measured using nanostructured systems of Au(2nm)/Cu(20nm)/Fe_3O_4(nanoparticles)/SiO_2/Si with varying the angle between magnetic field direction and substrate plane from 0° to 90°. The resulted maximum value of magnetoresistance was about 2 %.

DF 9.14 Tue 12:15 Poster A

^{57}Fe Mössbauer spectroscopy on ferrite nanoparticles — •Mathias Kraken[1], Jochen Litterst[1], Ilka-Marina Grabs[2], Ingke-Christine Masthoff[2], Isabel Christina Souza Dinóla[3], Julian Andres Munevar Cagigas[3], Wiliam Trujillo Herrera[3], and Elisa Maria Baggio Saitovitch[3] — [1]Institut für Physik der kondensierten Materie | TU Braunschweig | Germany — [2]Institut für Partikeltechnik | TU Braunschweig | Germany — [3]Centro Brasileiro de Pesquisas Físicas | Rio de Janeiro | Brazil

Due to its specific timescale, Mössbauer spectroscopy is highly suitable to investigate the dynamic properties of magnetic nanoparticles. The hyperfine magnetic spectra between the blocking temperature and very low temperatures may exhibit a broad variety of different shapes. Accordingly, to describe this rich behaviour a whole range of different, controversially discussed models can be found in literature (1-3).
We performed ^{57}Fe Mössbauer measurements on $ZnFe_2O_4$ nanoparticles, prepared by a non-aqueous sol gel method and characterized by different techniques. The spectra were taken on strongly and weakly interacting particles and the fits to the spectra with the different models are compared in order to gain information about their suitability.

(1) D.H. Jones et al., J. Magn. Magn. Mater. 78, 320 (1989).

(2) S. Mørup et al., J. Magn. Magn. Mater. 40, 163 (1983).

(3) S. Bocquet et al., J. Magn. Magn. Mater. 109, 260 (1992).

DF 9.15 Tue 12:15 Poster A

Preparing of $La_{1/3}Sr_{2/3}FeO_3$ targets for sputtering of thin films — •Thomas Breuer, Thomas Brueckel, Joerg Voigt, and Joerg Persson — Peter Gruenberg Institut PGI and Juelich Centre for Neutron Science JCNS, JARA-FIT, Forschungszentrum Juelich GmbH, 52425 Juelich, Germany

$La_{1/3}Sr_{2/3}FeO_3$ is a transition metal oxide (TMO) with a perovskite structure. It exhibits strong electronic correlations, visible e.g. in a Verwey metal-insulator transition accompanying the antiferromagnetic phase transition at about $T_C = 200\,K$.
While the material has been investigated extensively in bulk form, the aim of the present study is to clarify its properties as thin epitaxial films. We have prepared ceramic sputter targets of $La_{1/3}Sr_{2/3}FeO_3$ in a solid state reaction and characterized them by means of chemical analysis, powder x-ray diffraction and magnetic measurements by a Vibrating Sample Magnetometer on PPMS. The material tends to lose oxygen during calcination and sintering at temperatures above 600 K which was detected by thermogravimetric analysis. Significant changes in structure and magnetic response are being observed for oxygen deficits as low as 2 %. Finally, the progress in the preparation and characterization of thin epitaxial films will be reported.

DF 9.16 Tue 12:15 Poster A

The first principle study of Cu-based hybrids — •Pegah Zolfaghari[1], Gilles A de Wijs[1], and Robert A de Groot[1,2] — [1]Electronic Structure of Materials, Institute for Molecules and Materials, Faculty of Science, Radboud University Nijmegen, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands — [2]Solid State Materials for Electronics, Zernike Institute for Advanced Materials, Rijksuniversiteit Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands

Hybrids, organic-inorganic materials, in the perovskite-type layer structures with the general formula $(C_nH_{2n+1}NH_3)_2MCl_4$ in which $n = 0, 1, 2, ...$, and M represents a divalent transition metal ion, have been extensively studied in recent years. Among these series of hybrids, the copper compounds are the most interesting ones. Firstly, the divalent metal Cu^{2+} is a strong Jahn-Teller ion, as a result different structual transitions in these materials occur. Secondly, the magnetic intra-layer interactions are ferromagnetic.

The density functional (DFT) calculations were applied to study the $(NH_4)_2CuCl_4$ and $(C_2H_5NH_3)_2CuCl_4$ compounds. The magnetic and electronic properties were investigated. The calculations reveal that the compounds have a stable, layered ferromagnetic ground state that is consistent with experimental results.

DF 9.17 Tue 12:15 Poster A

Synthesis and magnetic properties of cobalt ferrite nanoparticles — •Morad F. Etier[1], Vladimir V. Shvartsman[1], Frank Stromberg[2], Joachim Landers[2], Heiko Wende[2], Fábio G. Figueiras[3], and Doru C. Lupascu[1] — [1]Institute for Materials Science, University of Duisburg-Essen, Essen, Germany — [2]Faculty of physics and Center for Nanointegration (CeNIDE) Duisburg-Essen, University of Duisburg-Essen, Duisburg, Germany — [3]Department of Physics, CICECO, University of Aveiro, Aveiro, Portugal

Cobalt ferrite is one of the most widely used materials in magnetic recording devices due to its high coercivity (about 5400 Oe), moderate magnetization (84 emu/g), and good chemical stability. Below Tc = 820 K cobalt ferrite is in a ferrimagnetic state. The magnetic properties of cobalt iron oxide nanoparticles mainly depend on the annealing temperature and particle size.

Nanoparticles of cobalt ferrite were successfully fabricated by the co-precipitation method. The crystal structure was confirmed by X-ray diffraction, the composition by energy dispersive spectroscopy, and phase changes by thermogravimetric differential thermal analysis. The particle morphology was analyzed by scanning electron microscopy. Magnetic properties were investigated by magnetometry and Mössbauer spectroscopy. Particle size is in the range of 24 to 44 nm. Both the particle size and agglomeration level are controlled by the amount of sodium hydroxide used. Dependence of remnant magnetization and coercive field on particle size is analyzed.

DF 9.18 Tue 12:15 Poster A

Magnetic and Electronic properties of Mn-stabilized Zirconia (MnSZ) — •Jan Zippel[1], Michael Lorenz[1], Anette Setzer[1], Holger Hochmuth[1], Pablo Esquinazi[1], Nikolai Sobolev[2], Alexandre Jacquot[3], and Marius Grundmann[1] — [1]Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentlaphysik II, Linnéstrasse 5, 04103 Leipzig, Germany — [2]Universidade de Aveiro, Departamento de Fisica, Campus de Santiago, 3810-193 Aveiro, Portugal — [3]Fraunhofer Institut für Physikalische Messtechnik, Heidenhofstrasse 8, D-79110 Freiburg, Germany

The possibility to combine both, the electron spin as a new degree of freedom and the electron charge offers opportunities for a new generation of devices. As recently predicted [1], MnSZ is proposed as a fer-

romagnetic semiconductor with a Curie temperature T_C above room temperature. As recently shown, a Mn related ferromagnetism has not been observed yet [2]. By applying an annealing step in oxygen defficient ambient at about $T_{\mathrm{ann}} \approx 700^\circ$ C to the MnSZ thin films grown by pulsed-laser deposition (PLD), we observe a ferromagnetic behavior in superconducting quantum interference device (SQUID) measurements at about $T = 60$ K. In addition, electron paramagnetic resonance (EPR) suggests a change of the Mn oxidation state from an EPR silent Mn^{3+} to Mn^{2+}. Seebeck-effect measurements verify a transition from p–type conductivity to n–type conductivity around 500 K. [1] S. Ostanin et *al.*, Phys. Rev. Lett. **98**, 016101 (2007). [2] J. Zippel et *al.*, Phys. Rev. B **82**, 125209 (2010).

DF 9.19 Tue 12:15 Poster A

The magneto-impedance of iron whiskers at low temperature — •Matthäus Langosch, Haibin Gao, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, P. O. Box 151150, D-66041, Saarbrücken, Germany

In order to understand all aspects of the AC transport behavior of a ferromagnetic material in an external magnetic field at low temperature, iron single crystals (iron whiskers) were grown as specific samples to investigate the magneto-impedance (MI) effect at 4.2 K. The MI measurements were performed as a function of the magnitude of the driving current and its frequency. The chosen frequencies were up to 100 kHz, where domain wall motion takes place and contributes to the MI effect. The measured low temperature impedance changes are on the order of hundreds of percent and are much higher than that at room temperature. This behavior can mainly be attributed to a large mean free electronic path on the one hand and the skin effect on the other hand.

DF 9.20 Tue 12:15 Poster A

Structural and magnetic analysis of Vanadates — •Christine Tölzer[1], Johanna Brand[1], Masahiko Isobe[2], Karsten Binder[1], Timo Taetz[3], María Teresa Fernández-Díaz[5], Angela Möller[3,4], Yutaka Ueda[2], and Markus Braden[1] — [1]II. Institute of Physics, University of Cologne — [2]Institute for Solid State Physics, University of Tokyo — [3]Institute of Inorganic Chemistry, University of Cologne — [4]Department of Chemistry and Texas Center for Superconductivity, University of Houston — [5]Institute Laue-Langevin, Grenoble

We present the analysis of three different Vanadates: $InCu_{2/3}V_{1/3}O_3$, $Rb_2V_8O_{16}$ and ZnV_2O_4. The layered compound $InCu_{2/3}V_{1/3}O_3$ is a representative of the quasi two-dimensional S=1/2 honeycomb lattice due to the ordering of Cu and V. A Néel-temperature near 38 K was deduced from anomalies in the magnetic susceptibility. We have studied the magnetic structure in $InCu_{2/3}V_{1/3}O_3$ by neutron diffraction on the high-flux powder diffractometer D20. A rise in scattering upon cooling indicates magnetic ordering to set in near the anomaly observed in the susceptibility. Furthermore, we discuss the charge and orbital ordering in $Rb_2V_8O_{16}$ and in ZnV_2O_4, as analysed by single-crystal x-ray diffraction as function of temperature.

DF 9.21 Tue 12:15 Poster A

Normal and anomalous Hall effect in $NbFe_2$ — •Sven Friedemann[1], Manuel Brando[2], William J Duncan[3], Andreas Neubauer[4], Christian Pfleiderer[4], and Malte Grosche[1] — [1]University of Cambridge, Cavendish Laboratory, JJ Thomson Avenue, CB3 0HE Cambridge, United Kingdom — [2]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Strasse 40, 01187 Dresden, Germany — [3]Department of Physics, Royal Holloway, University of London, Egham TW20 0EX, United Kingdom — [4]Physik Department E21, Technische Universität München, James-Franck-Strasse, D-85748 Garching, Germany

The intermetallic system $NbFe_2$ exhibits ferromagnetic and antiferromagnetic order, which can be suppressed by slight changes to the composition within the $Nb_{1-y}Fe_{2+y}$ homogeneity range. A quantum critical point (QCP) arises at slight Nb excess of about $y = 0.015$. In proximity to its QCP $NbFe_2$ exhibits non-Fermi-liquid behaviour, which makes this material the first clear candidate for a three dimensional ferromagnetic QCP in a clean transition metal compound at ambient pressure. We present Hall effect measurements on several single crystals chosen from the $Nb_{1-y}Fe_{2+y}$ solution series. The data are analysed in terms of anomalous and normal contributions to the Hall voltage. We find anomalous contributions arising from both Side Jump and Skew Scattering with distinct changes in their relative strength as a function of Nb content. The normal contribution reflects the electronic structure.

DF 9.22 Tue 12:15 Poster A

First principles studies of complex magnetism in Mn nanostructures on Fe(001) surface — •ricardo noboru igarashi[1], angela burlamaqui klautau[2], and helena maria petrilli[1] — [1]Instituto de Física, Universidade de São Paulo, CP 66318, 05315-970, São Paulo, SP, Brazil — [2]Faculdade de Física, Universidade Federal do Pará, Belém, PA, Brazil

The magnetic properties of Mn nanostructures on Fe(001) surface have been studied using the noncollinear first-principles RS-LMTO-ASA (Real-Space Linear Muffin Tin Orbital Atomic Sphere Approximation) [1] method within density functional theory. We have considered a variety of nanostructures such adsorbed wires, pyramids, flat and intermixed clusters of sizes varying from two and nine atoms. Our calculations of interatomic exchange interactions reveal the long range nature of exchange interactions between Mn-Mn and Mn-Fe atoms. We have found that the strong dependence of these interactions of the local environment and the effect of spin-orbit coupling lead to the possibility of realizing complex magnetic structures such as helical and half skyrmion.

[1] S. Frota-Pessôa, Phys. Rev. B 69, 104401 (2004); Phys. Rev. B 46, 14570 (1992); P. R. Peduto, S. Frota-Pessôa and M. S. Methfessel, Phys. Rev. B 44, 13 283 (1991).

DF 9.23 Tue 12:15 Poster A

Incorporation of N codopants in Co:ZnO investigated by X-ray absorption spectroscopy — •Daniel Schauries[1], Andreas Ney[1], Verena Ney[1], Fabrice Wilhelm[2], Andre Rogalev[2], and Flora Yakhou[2] — [1]Fakultät für Physik, Universität Duisburg-Essen, Lotharstr. 1, D-47057 Duisburg, Germany — [2]European Synchrotron Facility, 6 Rue Jules Horowitz, BP 220, 38043 Grenoble Cedex, France

p-doping of ZnO in general remains a grand challenge for material science. In particular p-type ZnO is of interest to investigate the perspectives for obtaining RT-ferromagnetism in p-type Co:ZnO.

We have grown Co:ZnO:N(0001) on sapphire substrates using reactive magnetron sputtering from Co/Zn targets at Co concentrations of 10, 15 and 20% and different Ar : O_2 : N_2 sputter gas compositions.

The structure was studied by synchrotron-based element specific X-ray absorption spectroscopy. All edges were measured with the electric field of the X-rays perpendicular and parallel to the c-axis to obtain X-ray Linear Dichroism (XLD). Subsequently all spectra for the Zn, Co, O and N-K-edge were simulated with FDMNES[1] to determinate the positions of the species. While Co only occupies Zn-sites, the situation turned out to be more complex for N — for low N_2-concentration in the sputter gas probably incorporated N_2 was formed, high N_2-levels also led to the formation of substitutional N atoms on O-sites.

The resulting magnetic properties of Co:ZnO:N will be discussed as well. We greatfully acknowledge financial support from the DFG through the Heisenberg Programme.

[1] Y. Joly, Phys. Rev. B **63**, 125120-125129 (2001).

DF 9.24 Tue 12:15 Poster A

Polarized Neutron Reflectometry of Rare-Earth Nitride Thin Films — •Sebastian Brück[1,2], David Cortie[2], Josh Brown[3], Thomas Saerbeck[2], Clemens Ulrich[1], Frank Klose[2], and James Downes[3] — [1]School of Physics, University of New South Wales, Sydney, Australia — [2]Australian Nuclear Science and Technology Organization, Lucas Heights, Australia — [3]Department of Physics, Macquarie University, Australia

Rare-earth monopnictides like HoN, DyN, or ErN are semiconductors with typical band gaps between 0.73 and 1.3eV. The fact that they exhibit ferromagnetic ordering at low temperatures makes them possible candidates for an intrinsically ferromagnetic semiconductor. Thin, polycrystalline rare-earth nitride films of 15 to 40nm thickness were grown onto c-plane sapphire substrates using low-energy ion assisted deposition. A temperature- and field-dependent polarized neutron reflectometry study in combination with SQUID magnetometry was carried out to characterize the magnetic properties of these films in a depth resolved way. The investigated samples show a homogeneous distribution of the magnetic moment throughout the film with ferromagnetic ordering temperatures comparable to the bulk materials. ErN and HoN films do not show an opening of the magnetic hysteresis loop even for the lowest measured temperature of T=2K. DyN on the other hand clearly shows a coercive field and remnant magnetization at 5K.

DF 9.25 Tue 12:15 Poster A

ZnO Metal Semiconductor Field Effect Transistor with magnetic channel — •Tim Kaspar, Danilo Bürger, Ilona Skorupa, Vicki Kühn, Artur Erbe, Manfred Helm, and Heidemarie Schmidt — Helmholtz-Zentrum Dresden-Rossendorf, P.O. Box 510119, 01314 Dresden, Germany

We focus on the development of transparent semiconductor spintronics devices. Our work is motivated by the observation of s-d exchange inducted spin polarization in magnetic ZnO:(Co, Mn) thin films below 50 K and related magnetoresistance effect [1]. Our aim is to control the conductance in ZnO Metal Semiconductor Field Effect Transistors (MESFET) with magnetic channel by external electrical AND magnetic fields. The magnetic ZnO:(Co, Mn) channel layers have been deposited by pulsed laser deposition on c-plane sapphire substrates. Gate, source, and drain contacts have been structured by optical lithography. The gate contact has been fabricated by reactive sputtering of Ag/Au [2]. Source and drain contacts have been fabricated from high conducting transparent ZnO. The characteristics of the ZnO-based MESFETs with magnetic channel in external perpendicular magnetic fields ranged from -1.8T to +1.8T are presented.

[1] Qingyu Xu, *et al.*, Phys. Rev. Lett. **101**, 076601 (2008)
[2] H.Frenzel *et al.*, Appl. Phy. Lett. **92**, 192108 (2008

DF 9.26 Tue 12:15 Poster A

Anomalous hysteretic Hall effect in a ferromagnetic, Mn-rich, amorphous Ge:Mn nano-network — •Danilo Bürger, Shengqiang Zhou, Marcel Höwler, Xin Ou, György Kovacs, Helfried Reuther, Arndt Mücklich, Wolfgang Skorupa, Manfred Helm, and Heidemarie Schmidt — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, P.O. Box 510119, 01314 Dresden, Germany

The read out of the magnetization state in magnetic semiconductors by electrical Hall resistance measurements makes it possible to use ferromagnetic semiconductors in nonvolatile memories. In a previous work [1], we fabricated ferromagnetic Ge:Mn by Mn ion implantation and pulsed laser annealing (PLA) and observed hysteretic Hall resistance below 10 K. By applying different PLA conditions we fabricated a percolating, Mn-rich, amorphous Ge:Mn nano-network with hysteretic Hall resistance up to 30K. This nano-network is embedded in crystalline Ge:Mn between 5 nm and 40 nm under the sample surface. We applied chemical and physical etching to confirm the contribution of the nano-network to the magnetic properties. The nano-network has a significant influence on the correlation between magnetism and anomalous Hall resistance. In the future such nano-networks may be used to spin-polarize free charge carriers in semiconductors at room temperature. [1] S. Zhou *et al.*, Phys. Rev. B **81**, 165204 (2010)

DF 9.27 Tue 12:15 Poster A

Optical and Magneto-optical Properties of ZnO(0001) Single Crystals Implanted with Fe and Co Ions — •Scarlat Camelia[1], Zhou Shengqiang[1], Gordan Ovidiu[2], Fronk Michael[2], Zahn R. T. Dietrich[2], Helm Manfred[1], Schmidt Heidemarie[1], and Salvan Georgeta[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany — [2]Semiconductor Physics, Chemnitz University of Technology, Germany

ZnO is a transparent wide-band-gap semiconductor which has been intensively investigated in the view of (magneto-) and (opto-)electronic applications. In this work the (magneto-)optical properties of unimplanted ZnO(0001) single crystals and single crystals implanted with ^{57}Fe and Co ions were investigated at room temperature by means of Raman spectroscopy, spectroscopic ellipsometry, and magneto-optical Kerr effect (MOKE) spectroscopy. The ZnO (0001) single crystals were coimplanted with ^{57}Fe and Co ions at 623 K with same fluence respectively. After implantation the samples were annealed in a high-vacuum furnace at 1073 K for different annealing time. The Raman spectra measured in resonance with an excitation energy of 3.82 eV exhibit higher order scattering by LO phonons. The increase in the ratio between the second and the first order phonon peak intensities for long annealing time can be correlated with a reduction in the number of defects and with improved crystallinity. The implanted ZnO crystals exhibit magneto-optical activity in two broad spectral ranges centered around 3 eV and around 4.3 eV, the strength of which also varies significantly with the annealing time.

DF 9.28 Tue 12:15 Poster A

Bipolar resistive switching at manganite/manganite interfaces — •Christin Kalkert, Jon-Olaf Krisponeit, Vasily Moshnyaga, Bernd Damaschke, and Konrad Samwer — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Bipolar resistive switching stands for remanent switching of resistivity by application of electric fields reversible by opposite polarities. This phenomenon is observed in a wide variety of perovskite materials and holds the potential of creating new resistive random access memory devices. $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) manganite films were prepared by using the metalorganic aerosol deposition technique. On Al_2O_3 substrates the manganite films show nanocolumnar growth with different growth orientations as determined by x-ray diffraction and TEM analysis. The films were structured by electron beam lithography into LSMO paths/bridges between larger LSMO contact areas; after a second lithography step Au/Cr films were deposited onto the contact areas. These structures show bipolar resistive switching, which can also be induced and probed by means of conductive AFM. The C-AFM measurements show that the switching takes place at the manganite/manganite interfaces, i.e. at the boundaries of the nanocolumns. The resistive switching of the structures and the C-AFM measurements are discussed in terms of a local structural transformation at the manganite/manganite interfaces. (APL 99, 132512, (2011))

Financial support by DFG via SFB 602, TPA2 and the Leibniz Program is ackowledged.

DF 9.29 Tue 12:15 Poster A

Ultrafast Spin-Lattice Coupling in Transition Metal Oxides — •Lena Maerten, André Bojahr, Marc Herzog, Daniel Schick, and Matias Bargheer — Insitut für Physik und Astronomie, Universität Potsdam, Germany

Understanding the interplay of the electronic, lattice and spin degrees of freedom in solids is essential for devising future nanoelectronic applications. Nanostructured transition metal oxides provide an ideal test ground for studying the interaction of the contributing subsystems on an ultrafast time scale.

We use femtosecond optical and infrared pump probe spectroscopy and time resolved x-ray diffraction techniques to investigate the electronic and lattice dynamics in $SrRuO_3/SrTiO_3$ and $(LaSr)MnO_3/SrTiO_3$ superlattices. Sub-picosecond buildup of magnetostrictive stress has been found in a $SrRuO_3/SrTiO_3$ nanolayer [1]. We show additional temperature- and fluence-dependent reflectivity data revealing further insight into the demagnetization process and discuss the coupling of the magnetic and structural degrees of freedom for the different materials by means of x-ray diffraction results.

[1]C. v. Korff Schmising et al., PRB 78, 060404 (2008)

DF 9.30 Tue 12:15 Poster A

Colossal Magnetoelastic Effects at the Phase Transition of (La, Pr, Ca)MnO_3 — •Markus Michelmann, Christoph Meyer, Vasily Moshnyaga, and Konrad Samwer — I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37707 Göttingen

A strong coupling of charge, spin and lattice degrees of freedom in perovskite manganites, i.e. (La, Pr, Ca)MnO_3, results from the competition between the ferromagnetic double exchange and charge/orbital ordering, promoted by the electron-phonon interaction. Therefore, the paramagnetic-ferromagnetic (PM-FM) phase transition is clearly reflected in the behavior of the elastic constants. Here, we report ultrasound velocity and attenuation in polycrystalline $(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3$ bulk samples (y = 0, 0.4, 0.5, 1) as a function of temperature, $T = 10 - 300$ K, and magnetic field, $B = 0 - 7$ T, with special focus on the hysteresis effects and metamagnetism at the 1st order PM-FM transition. Close to the Curie point modest magnetic fields, $B = 1 - 5$ T, induce a large increase of shear stiffness and a strong softening of bulk modulus by about 10%. A minimum in bulk modulus and a peak in longitudinal sound attenuation were observed at the phase transition and attributed to a coupling between the lattice and spin fluctuations. The magnitude of this softening is maximized at a certain temperature and magnetic field, indicating a critical end point of the magnetic transition. Support by Deutsche Forschungsgemeinschaft via SFB 602, TP A2 is acknowledged.

DF 9.31 Tue 12:15 Poster A

Magneto-optical Studies on Transition Metal doped Zinc Oxid — •Stephanie Jankowski[1], Sebastian Geburt[2], Carsten Ronning[2], and Wolfram Heimbrodt[1] — [1]Department of Physics and Material Science Center, Philipps- University Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Physikalisch-Astronomische Fakultät, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, D-07743 Jena,

Germany

We present the results of magneto photoluminescence on ZnO-bulk doped with the magnetic ions Co and Mn. The measurements have been performed in magnetic fields up to 7 Tesla in a temperature range 1.8-300 K. Zeeman spectroscopic in the excitonic region have been used to determine the g-factors of the samples. Normally the g-factor of II-VI diluted magnetic semiconductor is very high because of the Giant Zeeman effect. Even in case of transition metal doped ZnO surprisingly small Zeeman-splitting has been found. In comparison to other Mn- and Co-doped II-VI semiconductors the optical 3d intra-ionic transitions are very weak. The physical reasons for these phenomena will be discussed.

DF 9.32 Tue 12:15 Poster A

Microscopic and macroscopic studies on the magnetoelectric coupling in chiral multiferroics — Max Baum[1], •Jonas Stein[1], Simon Holbein[1], Thomas Finger[1], Navid Qureshi[1], Jeannis Leist[3], Joachim Hemberger[1], Petra Becker-Bohatý[2], Ladislav Bohatý[2], Götz Eckold[3], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Kristallographie, Universität zu Köln — [3]Institut für Physikalische Chemie, Universität Göttingen

In the chiral magnets $MnWO_4$ and $TbMnO_3$ ferroelectric polarisation is directly induced by the non-collinear magnetic structure. We present microscopic neutron scattering studies and macroscopic measurements of the ferroelectric polarisation and of the magnetic structure in these materials. Using a stroboscopic method the control of the chiral magnetism by an external electric field is analysed with polarised neutrons finding unexpectedly large relaxation times. Measurements of the pyrocurrent on $MnWO_4$ confirm these long time scales. In addition we discuss the magnetic excitations at the incommensurate zone centre of $MnWO_4$, a low energy mode should posses electromagnon character. The magnetic structure of $NaFe(WO_4)_2$ was studied by neutron diffraction. At zero magnetic field we find an incommensurate structure which transforms to commensurate order upon the application of moderate fields.

DF 9.33 Tue 12:15 Poster A

On the ferroelectric phase transition of boracites — •Michael Fechner and Nicola Spaldin — ETH Zurich, Department for Material Theory,CH-8093 Zurich, Switzerland

We present results of first-principles electronic structure calculations for the Cl and I boracites. The boracites[1] are a class of ferroelectric minerals with formula $Me_2B_7O_{12}X$, where Me is a bivalent metal (Fe, Co, Zn) and X a halogen (Cl, Br or I). All boracites are cubic at high temperature, and undergo a phase transition on cooling first to an orthorhombic phase and in some cases subsequently to a triclinic phase. Boracites with magnetic ions further develop magnetic ordering and become multiferroic. Here we investigate the mechanism for the ferroelectric phase transition from the cubic high symmetry phase to the orthorhombic ferroelectric intermediate and triclinic low temperature phase. Finally we found a dominant unstable phonon mode at the Γ point which drives the phase transition. However this mode couples with modes at the zone boundary making the boracites improper ferroelectrics.

[1] Nelmes, R., 1974. Structural Studies of Boracites - Review of Properties of Boracites. Journal Of Physics C-Solid State Physics, 7(21), pp.3840-3854.

DF 9.34 Tue 12:15 Poster A

XAS and XMCD of ultrathin Fe layers on $BaTiO_3$(001): Experiment and Theory — •Stephan Borek[1], Angelika Chassé[1], Guntram Fischer[1], Wolfram Hergert[1], Remya Kunjuvettil Govind[1], Karl-Michael Schindler[1], Vasili Hari Babu[2], Joachim Gräfe[2], Martin Welke[2], and Reinhard Denecke[2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg — [2]Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig

Promising candidates for switching the magnetization using voltages are multiferroic systems. As a model system we studied ultrathin Fe layers on $BaTiO_3$(001). Using x-ray absorption spectroscopy as a powerful method to investigate structural, electronic and magnetic properties simultaneously, the circular dichroism in x-ray absorption (XMCD) and x-ray absorption as such were used to determine the remanent magnetization as a function of film thickness. The onset of ferromagnetism at a temperature of 150 K was found for 5±1 layers. Using a Heisenberg-model in the framework of Monte-Carlo-Simulations shows that up to 3 monolayers the critical temperature is around 170 K. In addition the contribution of each layer could be separated using a fully relativistic multiple scattering formalism. Different magnetic structures and their impact on the spectroscopic properties, as well as the anisotropic behaviour of the multiferrroic systems have been investigated theoretically. The spin and orbital moments as obtained from the XMCD experiments and DMFT calculations will be compared.

DF 9.35 Tue 12:15 Poster A

Ferroelectricity and Magnetic Structure of Mn Moments in Multiferroic $GdMnO_3$ — •Enrico Schierle[1], Victor Soltwisch[1], Christoph Trabant[1,2], Alex Frano[1,3], Detlef Schmitz[1], Fabiano Yokaichiya[1,6], Andrej Maljuk[1,4], Dimitri Argyriou[1,5], and Eugen Weschke[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Germany — [3]MPI-FKF Stuttgart, Germany — [4]IFW, Dresden, Germany — [5]European Spallation Source, Lund, Sweden — [6]Laboratrio Nacional de Luz Sincrotron, Campinas-SP, Brasil

Orthorhombic $REMnO_3$ oxides can show strongly coupled ferroelectric (FE) and magnetic order, with FE polarization P induced by magnetic cycloids of the Mn spins[1,2]. However, from recent X-ray diffraction studies, there is growing evidence for a decisive role of ordering of the RE-4f moments as well and it seems that a large part of P can be explained by ionic displacements not necessarily connected with cycloidal magnetic order of Mn moments[3,4,5]. We employed Resonant Soft X-Ray Scattering at the Mn-$L_{2,3}$ resonance to prove the existence of a ferroelectric phase at the surface of $GdMnO_3$ even in zero external magnetic field and to examine its connection to the magnetic structure of the Mn moments in an element specific way.

[1] Kimura et al., Nature **426**, 55-58 (2003) [2] Kenzelmann et al., PRL **95**, 087206 (2005) [3] Schierle et al., PRL **105**, 167207 (2010) [4] Feyerherm et al., Journal of Physics: Conference Series **200**, 012032 (2010) [5] Walker et al., Science **333**, 1273 (2011)

DF 9.36 Tue 12:15 Poster A

Electronic and magnetic properties of $LuFe_2O_4$ — •Christine Derks[1], Karsten Kuepper[2], Manfred Neumann[1], Dharmalingam Prabhakaran[3], Stephen J. Blundell[3], Andrei Rogalev[4], and Fabrice Wilhelm[4] — [1]Fachbereich Physik, Universität Osnabrück, Germany — [2]Institut für Festkörperphysik, Universität Ulm, Germany — [3]Department of Physics, University of Oxford, United Kingdom — [4]ESRF, Grenoble, France

$LuFe_2O_4$ is a compound showing fascinating magneto electric coupling via charge ordering. Electronic and magnetic properties of the charge ordered phase of LuFe2O4 have been investigated by means of x-ray spectroscopic and theoretical electronic structure approaches [1]. Using hard x-ray radiation of the ESRF ID12 circular polarisation beamline, Fe K-edge and Lu L-edge spectra have been detected. The Fe K-edge spectra will be discussed in comparison to the former Fe L-edge spectra. The Lu L-edge spectra show very interesting XMCD signals from which a small magnetic moment could be deduced.

[1]Kuepper et al. Phys. Rev. B, Vol. 80, 22, 220409

DF 9.37 Tue 12:15 Poster A

Influence of the strength of the magnetoelectric coupling on the electric field induced magnetization reversal in a composite multiferroic chain — Paul P. Horley[1], Alexander Sukhov[2], Chenglong Jia[2], Eduardo Martinez[1], and •Jamal Berakdar[2] — [1]Centro de Investigacion en Materiales Avanzados (CIMAV S.C.), Chihuahua/Monterrey, 31109 Chihuahua, Mexico — [2]Institut für Physik, Martin-Luther Universität Halle-Wittenberg, 06120 Halle/Saale, Germany

A theoretical study of the multiferroic dynamics in a composite one-dimensional system consisting of unstrained $BaTiO_3$ multiferroically coupled to an iron chain is presented. The method [1] is based on the thermodynamical treatment of the magnetization and the polarization quantitatively described via the Landau-Lifshits-Gilbert and the Landau-Khalatnikov equations (both at T=0 K) coupled via an additional term in the total free energy. The coupling originates from the screening charge induced in the ferromagnet by the ferroelectric polarization in a very narrow interfacial layer. For real parameters corresponding to the rhombohedral phase of $BaTiO_3$ and for bcc iron and for a wide range of strengths of this coupling we predict the possibility of obtaining a well-developed hysteresis in the ferromagnetic part of the system induced by an external electric field. We also inspect the dependence of the reversal modes on the electric field frequency and

predict a considerable stability of the magnetization reversal for frequencies in the range of 0.5÷12[GHz]. [1] A. Sukhov *et al.,* J. Phys.: Cond. Matter **22**, 352201 (2010); Ferroelectrics (at press).

DF 9.38 Tue 12:15 Poster A

Electric field controlled manipulation of the magnetization in $BaTiO_3$ based ferroelectric/ferromagnetic hybrid structures — •Stephan Geprägs, Matthias Opel, Sebastian T. B. Goennenwein, and Rudolf Gross — Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching

Multiferroic materials, which simultaneously possess at least two long-range ordering phenomena in the same phase, have attracted widespread interest over the last years. In particular, the coexistence and cross-coupling of ferroelectric and ferromagnetic ordering in magnetoelectric multiferroics could offer the possibility to electrically read and write the magnetic state in future non-volatile memory cells. Unfortunately, these materials are scarce in nature. Attractive alternatives are composite material systems, in which ferromagnetic and ferroelectric compounds are combined. Such extrinsic multiferroic structures enable large and robust magnetoelectric effects at room temperature due to the elastic coupling between the ferroic constituents.

Here, we report on the electric field control of the magnetization in ferromagnetic/ferroelectric hybrid structures based on $BaTiO_3$ single crystals, using different materials as ferromagnetic layer, such as polycrystalline Ni and $Fe_{50}Co_{50}$ as well as epitaxial Fe_3O_4 and Sr_2CrReO_6 thin films. In these hybrid structures, reversible and irreversible changes of the magnetization as a function of the applied electric field were found, which are discussed in the framework of a theoretical model based on molecular dynamics simulations.

DF 9.39 Tue 12:15 Poster A

Interfacial effects on $[(SrMnO_3)_j/(LaMnO_3)_k]_N$ multilayers — •Markus Waschk, Paul Zakalek, Alexander Weber, and Thomas Brückel — Jülich Centre for Neutron Science JCNS-2 and Peter Grünberg Institut PGI-4, Forschungszentrum Jülich GmbH, D-52425 Jülich

On the search for new storage devices, the combination of ferroelectric and ferromagnetic properties in metal-oxide layers opens a wide field of new non-volatile memory devices, which show low energy consumption. Here we combine $LaMnO_3$ (LMO) and $SrMnO_3$ (SMO), which both are antiferromagnetic bulk insulators, while a multilayer stack behaves as ferromagnetic conductor for very small bilayer thicknesses. The ferromagnetism of the lower LMO layer is induced by the interface to the upper SMO layer. The influence is strongly dependent on the roughness of the interface, and was not yet observed in the opposite boundary. Our multilayers are grown epitaxially on $SrTiO_3$ (STO) (100) single crystals by an oxygen-assisted Molecular Beam Epitaxy System and alternatively, to compare both preparation methods, by a high pressure oxide sputtering system. Within our very smooth layers with interfacial roughness of the order of a unit cell we study the influence of the interface quality on the magnetic behaviour. We present the preparation method from first steps to a complex multilayer and the results of our in-house characterisation methods. Further we show our first results of a polarized neutron reflectometry study at D-17 of the ILL in Grenoble which show depth resolved the magnetic properties of the single layers and interfaces.

DF 9.40 Tue 12:15 Poster A

Fe-Cr cation ordering in PLD grown thin-films of multiferroic double perovskite Bi_2FeCrO_6 — •Vikas Shabadi, Philipp Komissinskiy, Mehran VafaeeKhanjani, Aldin Radetinac, and Lambert Alff — Institut für Materialwissenschaft, Technische Universität Darmstadt, Petersenstraße 23, 64287 Darmstadt, Germany

Co-existence of magnetism and ferroelectricity was theoretically predicted in the ordered double perovskite Bi_2FeCrO_6 [1]. We report epitaxial BFCO thin-films grown by pulsed laser deposition from a 20 % Bi-rich ceramic target on single crystal $SrTiO_3$(100) substrates. The degree of the Fe-Cr cation ordering in the BFCO films was comparatively calculated based on the X-ray diffraction patterns. The magnetic moments of the BFCO films were measured with a SQUID magnetometer and analyzed as a function of the Fe-Cr ordering. We believe that the discrepancies in the previously reported values of the magnetic moment of BFCO are connected to the varying degree of Fe-Cr cation ordering [2,3]. Further motivation has been derived from a recent experiment that achieved more than 90 % spontaneous B-site ordering in a similar Fe-Cr based double perovskite system [4].

[1] P. Baettig and N. A. Spaldin. Appl. Phys. Lett. 86, 012505 (2005)
[2] D. H. Kim et al. Appl. Phys. Lett. 89, 102902 (2006)
[3] R. Nechache, et al. J. Appl. Phys. 105, 061621 (2009)
[4] S. Chakraverty, M. Kawasaki et al. Phys. Rev. B 84, 064436 (2011)
The authors would like to acknowledge the support from DAAD.

DF 9.41 Tue 12:15 Poster A

Chemical solution deposition of multiferroic La0.7Sr0.3MnO3, BaTiO3 thin films prepared by ink plotting — •Anke Kirchner[1], Melis Arin[2], Petra Lommens[2], Xavier Granados[3], Susagna Ricart[3], Bernhard Holzapfel[1], and Isabel van Driessche[2] — [1]IFW Dresden, Institute for Metallic Materials, Helmholtzstr. 20, 01069 Dresden, Germany — [2]SCRiPTs, Department of Inorganic and Physical Chemistry, Ghent University, Krijgslaan 281 (S3), 9000 Ghent, Belgium — [3]Materials Science Institute of Barcelona, CSIC-ICMAB, Campus Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain

Ferroelectric BaTiO3 (BTO) as well as ferromagnetic La0.7SrMnO (LSMO) thin films were prepared by chemical solution deposition (CSD). Based on these, a multiferroic architecture stack of La0.7Sr0.3MnO3 / BaTiO3 layers was developed. Aqueous, environmentally friendly precursor solutions were formulated for both materials. These are used for ink plotting on SrTiO3 (100) substrates. Films were subjected to a subsequent thermal treatment at the corresponding crystallization temperature. The structural as well as the magnetic and electric properties are presented. The Curie temperature of the ferromagnetic LSMO layer with a film thickness of only 60 nm was determined to 360 K. The magnetization curve indicates a hysteresis loop with a saturation magnetization above 400 emu/cm3. The ferroelectric character of the BTO films was demonstrated by polarization curves.

DF 9.42 Tue 12:15 Poster A

Diffraction Anomalous Fine Structure of Ho_2PdSi_3 and $YMn_{2-\xi}Fe_\xi O_5$ — •Melanie Nentwich[1], Matthias Zschornak[1], Carsten Richter[1,2], and Dirk C. Meyer[1] — [1]TU Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Straße 23, 09596 Freiberg — [2]Hamburger Synchrotronstrahlungslabor HASYLAB at DESY

Diffraction Anomalous Fine Structure (DAFS) is a site-selective method for studying local electronic structures. As an advantage over X–ray Absorption Fine Structure (XAFS) it is possible to differentiate between atoms of the same kind but different Wyckoff positions which is especially useful for site–ordered mixed valence systems. Here, this method was applied to study the substitution of Mn atoms with Fe on the octahedral and pyramidal sites in $YMn_{2-\xi}Fe_\xi O_5$ [2]. Further, the *c*–ordering of Pd substitutes on Si sites according to a super structure proposal from F. Tang et al. [1] was investigated for the intermetallic compound Ho_2PdSi_3. Theoretical modelling was performed using the FDMNES code [3]. The measurements of the experimental data have been carried out at beamline E2 of DESY/HASYLAB Hamburg.

[1] F. Tang et al., Phys. Rev. B 84, 104105 (2011).
[2] F. Wunderlich et al., Phys. Rev. B 82, 014409 (2010).
[3] Y. Joly, Phys. Rev. B 63, 125120-125129 (2001).

DF 9.43 Tue 12:15 Poster A

Synthesis and characterisation of $BaTiO_3$ nanopowders and $CoFe_2O_4/BaTiO_3$ nanocomposites — •Yanling Gao, Morad Etier, and Doru C. Lupascu — Institute for Materials Science, University Duisburg-Essen, Universitätsstrasse 15, 45141 Essen, Germany

Multiferroic materials have drawn much attention, because they display the coexistence of ferroelectric and magnetic properties. In this study, we have succeeded in the synthesis and characterization of the $BaTiO_3$ nanocrystals by the low cost and straightforward autocombustion process of amorphous organic precursor. In the following, $CoFe_2O_4/BaTiO_3$ nanocomposites with core/shell structures were also obtained by using this process. The particles are systematically characterized by powder X-ray diffraction (XRD), scanning electron microscopy (SEM), thermogravimetric, differential thermal analyses (TGA/DTA), and infrared spectroscopy (IR). The XRD results confirm the presence of both the spinel and the perovskite phases. The SEM-EDX and the atomic force microscopy (AFM) micrographs of $CoFe_2O_4/BaTiO_3$ show two-phase composite nanostructures of a cobalt ferrite core coated with a $BaTiO_3$ shell. The weight fraction of

$CoFe_2O_4$ and the size of nanocomposites are the keys to the dielectric and magnetic properties of $CoFe_2O_4/BaTiO_3$ nanocomposites.

DF 9.44 Tue 12:15 Poster A

Topology of spin polarization of the 5d states on W(110) and Al/W(110) surfaces — •Artem G. Rybkin[1], E. E. Krasovskii[2,3,4], D. Marchenko[5], E. V. Chulkov[2,4,6], A. Varykhalov[5], O. Rader[5], and A. M. Shikin[1] — [1]St. Petersburg State University — [2]University of the Basque Country, San Sebastián — [3]IKERBASQUE Bilbao — [4]Donostia International Physics Center — [5]Helmholtz-Zentrum Berlin — [6]Materials Physics Center, CSIC-UPV/EHU, San Sebastián

The spin polarization of W(110) and Al/W(110) surfaces is studied by spin- and angle-resolved photoemission. On both surfaces distinct $E(\mathbf{k}_\parallel)$ dispersions are identified with an unusual topology: a single spectral branch is spin polarized antisymmetrically relative to the $\bar{\Gamma}$ point, and two spin-polarized branches cross at $\bar{\Gamma}$. Based on *ab initio* theory coupled with one-step photoemission calculations, we show that the measured spin polarization is a property of the ground state and identify the effect as the counterpart of the recently discovered Rashba-polarized bulk states but with a distinct non-Rashba topology. We address also the question of topological protection.

DF 9.45 Tue 12:15 Poster A

STM studies on the ternary topological insulator $PbBi_4Te_7$ — •Andreas Eich, Alexander Ako Khajetoorians, Julian Hagemeister, Oswald Pietzsch, Jens Wiebe, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, D-20355 Hamburg, Germany

Topological insulators are a new class of materials with a bulk band gap like an ordinary insulator but exhibit a gapless surface state where the spin and momentum are locked. This topological surface state which results from a combination of spin-orbit interactions and time-reversal symmetry exhibits exotic spin-dependent transport phenomena at the surface. Nevertheless, the electronic properties of these surface states can be influenced by adsorbates. By adding a third component to a binary topological insulator it is also possible to influence both the energetic position of the Dirac cone and the surface state localization. Here we show STM measurements of the structure of a ternary topological insulator, namely $PbBi_4Te_7$. It has a hexagonal unit cell and contains five-layer (5L) and seven-layer (7L)-blocks with the atomic layer sequence, Te-Bi-Te-Bi-Te (5L) and Te-Bi-Te-Pb-Te-Bi-Te (7L). Theory predicts that not only the position of the Dirac cone relative to the Fermi energy is changed but that the surface states are localized in the 7L-block, leading to buried surface-states in the case of a 5L-terminated surface. We review the growth properties of this crystal and comment on the topological properties of these layers.

DF 9.46 Tue 12:15 Poster A

Bose-Hubbard model on two-dimensional line graphs — •Johannes Motruk and Andreas Mielke — Institut für Theoretische Physik, Ruprecht-Karls-Universität Heidelberg, Philosophenweg 19, D-69120 Heidelberg

We investigate the positive hopping bosonic Hubbard Model on line graphs of finite 2-connected planar bipartite graphs. The model on these lattice geometries exhibits flat bands and the single- as well as many-particle ground states are highly degenerate. Using notions from graph theory, we are able to give a basis for the space of many-particle ground states. The particles in these states are localized on vertices of the line graph which are edges of the original graph belonging to edge-disjoint cycles. This construction works up to a certain critical filling factor at which the cycles are close-packed. We rigorously show the linear independence of these states and prove that they span the space of many-particle ground states.

Furthermore, we establish that the entropy per lattice site in the ground state with constant (except critical) filling factor remains finite in the thermodynamic limit. Some of our findings can be applied to spin models of quantum antiferromagnets at high fields on the considered lattices.

DF 9.47 Tue 12:15 Poster A

Growth, Annealing and Characterization of $Sr_3Fe_2O_{7-\delta}$ — •Darren Peets[1], Junghwa Kim[1], Andrey Maljuk[1,2], Chengtian Lin[1], and Bernhard Keimer[1] — [1]MPI-FKF, Heisenbergstr. 1, D-70569 Stuttgart — [2]IFW Dresden, Helmholtzstr. 20, D-01069 Dresden

Iron(IV)- and ruthenium(IV)-containing perovskite-related phases have proven rich in novel physics. $SrFeO_{3-x}$ exhibits a wide variety of unusual magnetic phases, from five distinct types of helical magnetism at $x = 0$ [1] to a phase with frustrated, disordered Fe^{4+} moments at $x = 0.25$ [2]. The Ru-based intergrowth phase $Sr_3Ru_2O_7$ exhibits metamagnetic quantum critical points in field. However, the magnetic phase diagram of its Fe^{4+} analogue $Sr_3Fe_2O_{7-\delta}$ remains largely unexplored. We report the crystal growth, oxygen annealing, and characterization of large single-crystalline samples of $Sr_3Fe_2O_{7-\delta}$ suitable for neutron diffraction experiments. This work lays the foundation for comprehensive doping-dependent studies of $Sr_3Fe_2O_{7-\delta}$'s magnetic phase diagram and magnetic excitations.

[1] S. Ishiwata *et al.*, Phys. Rev. B **84**, 054427 (2011)
[2] M. Schmidt *et al.*, J. Phys.: Condens. Matter **15**, 8691 (2003)
[3] R.A. Borzi *et al.*, Science **315**, 214 (2007)

DF 9.48 Tue 12:15 Poster A

Finite-temperature density-functional theory of the Hubbard model — •Tobias Müller and Gustavo Pastor — Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel

The finite temperature properties of the Hubbard model are investigated in the framework of lattice density-functional theory (LDFT). The single-particle density matrix γ_{ij} with respect to the lattice sites is considered as the basic variable of the many-body problem. Following Mermin's theorem the free energy $F = E - TS = K + W - TS$ at temperature T is regarded as a functional of γ, where $K[\gamma]$, $W[\gamma]$ and $S[\gamma]$ stand for the kinetic-energy, Coulomb-energy and entropy functionals, respectively. A finite-temperature extension of Levy's constraint search approach is formulated. In this framework exact numerical results for W and S are obtained as a function of the nearest-neighbor γ_{ij} and T for different system sizes at half-band filling. The properties of these functionals are discussed in some detail. On the basis of this analysis we propose a simple explicit approximation to $W[\gamma]$ and $S[\gamma]$ which is relevant to arbitrary lattices. The method is finally applied to one-dimensional systems and the accuracy of the derived equilibrium properties is discussed

DF 9.49 Tue 12:15 Poster A

Green function of the single-site full-potential scattering problem including scalar-relativistic and spin-orbit effects — •David Bauer, Phivos Mavropoulos, Rudolf Zeller, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich

We present a method for the solution of the scalar-relativistic equation for a finite-range non-spherical potential and with the option of including spin-orbit coupling. Our scope is to determine the Green function for the single-site scattering problem, which is used in the multiple-scattering Korringa-Kohn-Rostoker Green function method for electronic structure calculations of impurity atoms embedded in a crystalline host.

The Green function can be written in a semi-separable form where the regular and irregular radial solutions of the scalar-relativistic operator are used. Also the right- and left-hand-side solutions are needed, which are not necessarily identical and can differ for example when including spin-orbit coupling as a pertubative term. The radial functions are calculated by a direct solution of a generalized Lippmann-Schwinger (LS) integral equation by employing a Chebyshev expansion. To save computational time, we proceed in a two step approach. First a LS equation is solved for the spherically symmetric case. The result is used to determine the Green function of the spherical problem, which in a second step is used in a new LS equation that includes non-spherical and spin-orbit terms. The latter has a special structure which allows a reduction of the computational time.

DF 9.50 Tue 12:15 Poster A

Micromagnetic Simulations of Spin Dynamics in Magnetic Nanodots — •Robert Rückriem[1], Philipp Krone[1], Thomas Schrefl[2], and Manfred Albrecht[1] — [1]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]St. Pölten University of Applied Science, St. Pölten, Austria

Micromagnetic simulations were performed to investigate the spin dynamics in a single magnetic nanodot varying diameter ($50-150$ nm), thickness ($5-20$ nm), saturation magnetization ($0.5-2.0$ T) and uniaxial anisotropy ($0-250$ kJ/m^3). Using a finite element based three step simulation technique, the spatial distribution of excited spin waves as well as their frequency spectra was obtained. The occurring spin wave modes were identified as edge modes which are strongly influenced by demagnetizing field effects [1] and center modes which oscillate in the

whole nanodot. By changing the magnetic and geometric parameters of the nanostructure, the precession frequency can be tuned which is important for magnetic engineering for instance in the field of microwave assisted magnetic recording [2].

[1] J. Jorzick, S. O. Demokritov, B. Hillebrands, M. Bailleul, C. Fermon, K. Y. Guslienko, A. N. Slavin, D. V. Berkov and N. L. Gorn, Phys. Rev. Lett. 88, 047204 (2002)

[2] J.-G. Zhu, X. Zhu, Y. Tang, IEEE Trans. Magn. 44, 125 (2008)

DF 9.51 Tue 12:15 Poster A

Pairs of diverging-converging spin vortices in biquadratically interlayer exchange coupled elements — •Sebastian Wintz[1], Christopher Bunce[1], Anja Banholzer[1], Thomas Strache[1], Michael Körner[1], Sibylle Gemming[1], Artur Erbe[1], Jeffrey McCord[2], Jörg Raabe[3], Christoph Quitmann[3], and Jürgen Fassbender[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Christian-Albrechts-Universität zu Kiel, Kiel, Germany — [3]Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland

Spin structures have been a relevant topic of magnetism research for many years. In particular, magnetic vortices have attracted much attention, due to their non-trivial topology and the various dynamic modes they exhibit [1]. A magnetic vortex consists of a planar, flux-closing magnetization curl that turns out of the plane in the central nanoscopic core. For a single layer structure, the curl's radial components typically cancel each other out. Recent investigations show that this holds also true for multilayer vortex systems comprising bilinear interlayer exchange coupling (IEC) [2]. In this contribution we report on pairs of diverging-converging spin vortices occurring in biquadratically coupled systems. Using magnetic x-ray microscopy we directly observe that the individual vortices of such pairs possess a residual radial magnetization component. From this $\nabla \mathbf{M}_{xy} \neq 0$, an additional perpendicular magnetization divergence $\nabla \mathbf{M}_z$ is analytically deduced. We compare our continuous model with discrete micromagnetic simulations. [1] S.-B. Choe et al., Science 304, 420 (2004). [2] S. Wintz et al., Appl. Phys. Lett. 98, 232511 (2011).

DF 9.52 Tue 12:15 Poster A

Structural, electronic, and magnetic properties of CoO/Ni interfaces — •Udo Schwingenschlögl, Sergiy Grytsyuk, and Fabrizio Cossu — KAUST, PSE Division, 23955-6900 Thuwal, Kingdom of Saudi Arabia

We study the CoO/Ni interface. Since the lattice mismatch of Ni with respect to CoO is about 21% we use a large supercell for our first-principles calculations, which reduces the lattice mismatch to 0.8%. We investigate the structural, electronic, and magnetic properties of two CoO/Ni interfaces: (1) An O layer mediates the coupling between Ni and Co and (2) direct Ni-Co contact. Our results indicate that the magnetization is reduced by 19% in the first case, while in the second case it increases by 106% as compared to bulk Ni. The magnetic moments of the Ni atoms are larger if the exchange coupling is mediated by O atoms, while for direct contact with the Co atoms they become smaller than in the bulk. The Co 3d local density of states of the second interface shows surprisingly small deviations from the corresponding bulk results, although the first coordination sphere is no longer octahedral.

DF 9.53 Tue 12:15 Poster A

Exchange-bias effects in Co/$YMnO_3$ bilayer: Magnetization and magneto-transport measurements — •J. Barzola-Quiquia, A. Lessig, C. Zandalazini, G. Bridoux, and P. Esquinazi — Division of Superconductivity and Magnetism, University of Leipzig, D-04103 Leipzig, Germany

The exchange bias effects in a bilayer composed by the antiferromagnetic o-$YMnO_3$ and ferromagnetic Co thin films have been investigated through SQUID magnetometry and magneto-transport measurements. Magnetization hysteresis loops and magneto-transport properties show pronounced asymmetries in the field and magnetization axis. Both exchange bias parameters, the exchange bias field $H_E(T)$ and the magnetization shift $M_E(T)$, vanish around the Néel temperature $T_N \simeq 45$ K. The magnetization shift is also measured by a shift in the longitudinal and Hall resistances showing a similar temperature dependence as the one obtained from magnetization measurements. Because the o-$YMnO_3$ film is highly insulating, our results demonstrate that the M_E shift is related to the pinned moments within the ferromagnetic Co layer at the interface.

DF 9.54 Tue 12:15 Poster A

Perpendicular exchange bias in ferrimagnetic spin valves — •Radu Abrudan[1], Ilie Radu[2], Detlef Schmitz[3], Hartmut Zabel[1], and Florin Radu[3] — [1]Institut für Experimentalphysik/Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Radboud University Nijmegen, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen,The Netherlands — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Albert-Einstein-Strasse 15, 12489 Berlin, Germany

Exchange bias effect refers to the shift of the hysteresis loop of a ferromagnet which is in direct contact to an antiferromagnet. For applications in spintronics a robust and tunable EB effect is required. We present experimental evidence for perpendicular EB in ferrimagnetic spin valves in a $DyCo_5$/Ta/$Fe_{76}Gd_{24}$ prototype trilayer, where the $DyCo_5$ alloy plays the role of a hard ferrimagnet and the Fe_76Gd_{24} is a soft ferrimagnet. Taking advantage of the tunability of the exchange coupling between the ferrimagnetic layers by means of thickness variation of an interlayer spacer, we show that perpendicular exchange bias can be induced with desirable absolute values at room temperature with no field cooling procedure. Moreover, the shift of the hysteresis loop can be reversed with relatively low magnetic fields of several hundred Oersteds. This flexibility in controlling a robust perpendicular EB at room temperature may be of crucial importance for applications.

DF 9.55 Tue 12:15 Poster A

Renormalization of exchange coupling parameters in systems with coexisting strong and induced magnetic moments — •Phivos Mavropoulos, Marjana Ležaić, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich

In magnetic systems with coexisting strong and induced (weak) magnetic moments, it is often the case that the magnetic excitations change the direction and magnitude of the weak moments but only the direction of the strong moments. It is also often the case that the energy landscape can be parametrised by a quadratic dependence on the weak-moments magnitude in addition to a Heisenberg expression for the strong-moments direction. We show that under these conditions the weak moments can be completely eliminated as degrees of freedom in favour of renormalized exchange coupling parameters among the strong moments. We further show that this renormalization is also valid at elevated temperatures. The thermodynamic properties (including all correlation functions) of the full system, where the strong and weak moments are independent degrees of freedom, can be derived from the correlation functions of the renormalized system, where only the strong moments are accounted for as degrees of freedom. A prerequisite for the latter theorem is a quadratic measure in the phase space of the weak moments. The theorem justifies certain schemes for the derivation of exchange parameters and can also be of practical use for reducing the numerical load in calculations.

DF 9.56 Tue 12:15 Poster A

Coupling Single Molecule Magnets to Ferromagnetic Substrates — Alberto Lodi Rizzini[1], Cornelius Krull[1], •Timofey Balashov[1], Jerald Kavich[1], Aitor Mugarza[1], Piter Miedema[2], Pardeep Thakur[3], Violetta Sessi[3], Svetlana Klyatskaya[4], Mario Ruben[4], Sebastian Stepanow[5], and Pietro Gambardella[1] — [1]ICN, Barcelona, Spain — [2]Utrecht University, Utrecht, The Netherlands — [3]ESRF, Grenoble, France — [4]Institute of Nanotechnology, KIT, Germany — [5]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

We investigate the interaction of $TbPc_2$ single molecule magnets (SMMs) with ferromagnetic Ni substrates. Using element-resolved x-ray magnetic circular dichroism, we show that $TbPc_2$ couples antiferromagnetically to Ni films through ligand-mediated superexchange. This coupling is strongly anisotropic and can be manipulated by doping the interface with electron acceptor or donor atoms. We observe that the relative orientation of the substrate and molecule anisotropy axes critically affects the SMM magnetic behavior. $TbPc_2$ complexes deposited on perpendicularly magnetized Ni films exhibit enhanced magnetic remanence compared to SMMs in the bulk. Contrary to paramagnetic molecules pinned to a ferromagnetic support layer, we find that $TbPc_2$ can be magnetized parallel or antiparallel to the substrate, opening the possibility to exploit SMMs in spin valve devices.

DF 9.57 Tue 12:15 Poster A

Zero bias anomalies and magnon excitation in tunnel junctions with magnetic and nonmagnetic electrodes — •Volker Drewello, Zoë Kugler, Günter Reiss, and Andy Thomas —

Universität Bielefeld, Fakultät für Physik, Dünne Schichten und Physik von Nanostrukturen, Universitätsstr. 25, 33615 Bielefeld

In order to understand the tunneling spectra of magnetic tunnel junctions, tunnel junctions are fabricated in which one or both ferromagnetic electrodes were replaced by non-magnetic metal (tungsten). The bias dependence of these junctions is investigated with high accuracy by inelastic electron tunneling spectroscopy. Both types of junctions exhibit a zero bias anomaly that is different in size and sign compared to those of magnetic tunnel junctions, that is, junctions with two ferromagnetic electrodes. A pronounced difference is also found depending on the material that the electrons tunnel into, which is attributed to the excitation of magnons.

DF 9.58 Tue 12:15 Poster A

Electrical characterization of nanoscaled CoFeB|MgO|CoFeB-based magnetic tunneljunctions (MTJs) for thermal spin-transfer-torque (TST) — •Johannes Christian Leutenantsmeyer[1], Marvin Walter[1], Vladyslav Zbarsky[1], Patrick Peretzki[2], Henning Schuhmann[2], Michael Seibt[2], and Markus Münzenberg[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen — [2]IV. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen

MTJs are of general interest because of their quantum mechanical properties such as the tunnel-magnetoresistance (TMR), spin-transfer-torque and the recently measured magneto Seebeck effect.

Here we present the studies about our nanoscaled MTJs. The junctions are grown in UHV at base pressures around 5×10^{-10} mbar. The thin films are deposited by magnetron sputtering (Ta, CoFeB) and E-Beam evaporation (MgO, Ru). After annealing, the samples are patterned with bondpads via optical lithography, which enable us to contact sub-micron-scaled junctions. The MTJ itself is written by e-beam lithography and etched by argon-ion milling. With a high resolution e-beam resist, we reach a junction size of approximately 50 nm. The smaller junctions require the transition to thinner barriers (down to 3 monolayers), which we develop for the observation of new phenomena, like the theoretically predicted TST. Characterization shows TMR of up to 230% and large magneto Seebeck effect.

We gratefully acknowledge the funding of Deutsche Forschungsgemeinschaft through SFB 602 and SPP SpinCaT.

DF 9.59 Tue 12:15 Poster A

Spin transport and tunnel magnetoresistance of MgO-based magnetic tunnel junctions with different CoFeB compositions — •Vladyslav Zbarsky[1], Marvin Walter[1], Gerrit Eilers[1], Markus Münzenberg[1], Patrick Peretzki[2], Michael Seibt[2], and Johannes Leutenantsmeyer[1] — [1]I. Phys. Inst., Universität Göttingen, Germany — [2]IV. Phys. Inst., Universität Göttingen, Germany

The optimization of MTJs is necessary for increasing the TMR and therefore is very important for the production of MRAM devices. The quality of the tunnel barrier of our CoFeB/MgO/CoFeB MTJs is essential for getting high TMR. For this reason we minimized the roughness of MgO layer on the TMR. Another important parameter which we could optimize is the choice and preparation of the buffer layer. For example we compared two sorts of Ta buffer layers: prepared via magnetron sputtering and via e-beam evaporation. Already by optimizing these two parameters we could increase the TMR from 80% to above 220%. The next important step is further optimization of annealing parameters, because annealing influences the crystallisation behaviour of our MTJs. In this case, we investigate the influence of the annealing temperatures and annealing duration on the TMR. For the magneto-Seebeck effect a strong dependence on the choice of CoFeB composition is theoretically predicted. A change in the composition is of strong interest since the Fe to Co ratio gradually tunes the Fermi level by electron doping. In this context, we investigate the behaviour of TMR and spin transport for different CoFeB alloys.

DF 9.60 Tue 12:15 Poster A

Domain wall dependent magnetoresistance at zero field in electromigrated ferromagnetic nanocontacts. — •Mohamad-Assaad Mawass[1,5], Robert M. Reeve[1], Jakoba Heidler[2], Jan Rhensius[2,3], Laura J. Heyderman[2], Regina Hoffmann[4], André Bisig[2,3], and Mathias Kläui[1,2,3] — [1]Johannes Gutenberg-Universität Mainz, Mainz, Germany — [2]Paul Scherrer Institut, Villigen, Switzerland — [3]Universität Konstanz, Konstanz, Germany — [4]Physikalisches Institut and DFG-Center for Functional Nanostructures, Karlsruhe Institute of Technology, Karlsrue, Germany — [5]Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany

Magnetotransport measurements of magnetic nanocontacts have been studied with the aim to understand the interactions between spin-polarized charge carriers and magnetization on the nanoscale. Here, we study the evolution of magnetoresistance (MR) in electromigrated ferromagnetic break junctions obtained in clean ultra-high vacuum (UHV) conditions. While previously permalloy (Ni80Fe20) nanocontacts with variable constriction width have been investigated [A. Patra et al., PRB 82, 134447 (2010)], the question of the influence of the alloy nature on the observed MR effects remains. The in-situ controlled electromigration of notched half ring structures under UHV conditions for pure Ni and Fe contacts was investigated and similarly large effects could be observed. In particular, large MR effects at remanence are found in contacts that approach the atomic limit. Additionally, our measurements show a sign-change of the MR at low conductance levels and this is compared to recent theoretical predictions.

DF 9.61 Tue 12:15 Poster A

Anomalous Hall effect as a Fermi surface property — •Alexander Mook[1], Falko Pientka[1,2], Ingrid Mertig[1,3], and Peter Zahn[1] — [1]Institut für Physik, Martin-Luther-Universität, Von-Seckendorff-Platz 1, D-06120 Halle — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle — [3]Fachbereich Physik, Freie Universität, D-14195 Berlin

Already Haldane has shown in a seminal paper that the intrinsic anomalous Hall conductivity can be expressed as an integral over the Fermi surface as expected for a Fermi liquid property [1].

The anomalous Hall conductivity can be expressed either by a volume integral of the occupied states in the Brillouin zone or a Fermi surface integral with a thorough treatment of the Brillouin zone boundaries. We implemented both methods and applied them to a tight-binding Hamiltonian including exchange splitting and spin-orbit coupling.

Our investigations show that both results agree well. Details of the integration procedure have to be optimized to obtain a satisfying agreement for cases where avoided band crossings occur close to the Fermi level. The surface integration replaces the time consuming volume integration over the Fermi sea [2]. The method is applicable to advanced ab initio electronic structure schemes which provide besides the band energies also the Berry curvature.

[1] F. D. M. Haldane, *Phys. Rev. Lett.* **93**, 206602 (2004). [2] M. Gradhand, D. V. Fedorov, F. Pientka, P. Zahn, I. Mertig, and B. L. Göyrffy, *Phys. Rev. B* **84**, 075113 (2011).

DF 9.62 Tue 12:15 Poster A

Structural, electronic and transport properties of platinum-based chains: an ab initio study — •Ilia Sivkov, Kun Tao, and Valeri Stepanyuk — Max-Planck-Institut für Mikrostrukturphysik Weinberg 2, D-06120 Halle, Germany

We have investigated the structural, electronic and magnetic properties of platinum-based chains. Both pure platinum chains and chains with 3d impurities have been considered. The calculations of these properties were performed using methods based on the density functional theory.We show that the magnetic anisotropy energy of such chains strongly depends both on their shape, and on the impurities involved. Furthermore, transport calculations based on the non-equilibrium Green's function formalism have been performed.

DF 9.63 Tue 12:15 Poster A

Magnetic and transport properties of a series of dinuclear Nickel(II) complexes — •Claudia Loose[1], Torsten Hahn[1], Jens Kortus[1], Jochen Lach[2], and Berthold Kersting[2] — [1]TU Bergakademie Freiberg, Fakultät für Chemie und Physik — [2]TU Leipzig, Fakultät für Chemie und Mineralogie

Using first-principle density functional theory (DFT) we examined four different dinucklear Nickel(II) complexes [1] in order to obtain the electronic and magnetic structure with a special focus on spin-dependent transport through these molecules.

We compare results from different exchange correlation functionals (PBE/B3LYP) as implemented in two different packages (NRL-MOL/ORCA). Furthermore we investigate the transport properties of those complexes using methods of the non equilibrium Green's function formalism (NEGF).

[1] Coord. Chem. Rev. 253 (2009) 2244 - 2260

DF 9.64 Tue 12:15 Poster A

Optimization of spin-valve structures for spin-pumping ex-

periments — •Christian Swoboda, Nils Kuhlmann, Andreas Vogel, Toru Matsuyama, and Guido Meier — Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg, Jungiusstrasse 11, 20355 Hamburg, Germany

In recent years, high-frequency phenomena of magnetic nanostructures have been studied intensively since they are expected to provide new technological applications as well as fundamental understanding of spin dynamics. Currently, the combination of magnetization dynamics and spin transport, the spin-pumping effect [1, 2], is of great interest. First experimental results including the detection of pure spin currents have been presented [3]. The aim of our work is to build an all-metal lateral spin-valve [4], where the spins are injected into an adjacent normal-metal via a ferromagnet with precessing magnetization at ferromagnetic resonance (spin-pumping). The lateral spin-valve device enables to detect and to quantify the pure spin current via a second ferromagnet. Besides the basic concept of a lateral spin-valve device operated by spin-pumping, we present a detailed study of the magnetization dynamics of the ferromagnetic electrodes. We optimized geometry and center-to-center distance of the electrodes in order to enhance the spin-pumping efficiency.

[1] Y. Tserkovnyak et. al., PRL 88, 117601 (2002); [2] A. Brataas et. al., PRB 66, 060404 (2002); [3] M.V. Costache et. al., PRB 78, 064423 (2008); [4] A. Vogel et. al., APL 94, 122510 (2009)

DF 9.65 Tue 12:15 Poster A

Spin density distribution and Hanle lineshapes of injected spins into n-GaAs — •Bernhard Endres, Mariusz Ciorga, Robert Wagner, Sebastian Ringer, Martin Utz, Dominique Bougeard, Dieter Weiss, Christian H. Back, and Günther Bayreuther — Universität Regensburg

Spin extraction into a ferromagnetic GaMnAs contact from an n-GaAs channel across an Esaki diode structure was measured by cross-sectional imaging of the spin polarization in GaAs [1,2]. The resulting spin density distribution in the 1 μm thick GaAs channel shows a strong bias dependence with the maximum polarization at the contact edge opposite to the maximum charge current. This behavior cannot be described by a frequently used one-dimensional model whereas two-dimensional numerical simulations of the electron drift and spin diffusion reproduce the observed distribution quite well. Even at the nominally field-free contact edge electron drift must be taken into account because of the inhomogeneous current density. As a consequence, if Hanle measurements are fitted with a one-dimensional drift-diffusion function as usually done they yield spin lifetimes which may strongly depend on the distance to the contact and the applied bias voltage. In contrast, a two-dimensional fit including the nonuniform current density provides spin lifetimes nearly independent of bias and contact distance. The remaining variations can be explained by electric fields around the contact area. [1] P. Kotissek et al., Nature Phys. 3, 872 (2007) [2] B. Endres et al., J. Appl. Phys. 109, 07C505 (2011)

DF 9.66 Tue 12:15 Poster A

Fe_3O_4/ZnO: A high-quality magnetic oxide-semiconductor heterostructure by reactive deposition — •Ozan Kirilmaz[1], Sebastian Brück[1,2], Markus Paul[1], Andreas Müller[1], Eberhard Goering[3], Jo Verbeeck[4], He Tian[4], Michael Sing[1], and Ralph Claessen[1] — [1]Experimentelle Physik 4, Universität Würzburg, D-97074 Würzburg, Germany — [2]University of New South Wales, School of Physics, Sydney NSW 2052, Australia — [3]Max Planck Institute for Intelligent Systems, D-70569 Stuttgart, Germany — [4]Electron Microscopy for Materials Science, University of Antwerp, 2020 Antwerp, Belgium

Magnetite (Fe_3O_4) is ranked among the most promising materials to be used as a spin injector into a semiconducting host. We demonstrate epitaxial growth of Fe_3O_4 films on ZnO which presents a further step for polarized spin injection into semiconductors. Regarding volume properties of the films, X-ray photoelectron spectroscopy evidences that the iron-oxide is phase-pure and stoichiometric magnetite. Diffraction measurements indicate highly oriented epitaxy and complete structural relaxation. The magnetic behavior shows a slow approach to saturation at high fields in comparison with bulk crystals. The typical (111) surface structure of Fe_3O_4 is observed already at the early growth stage. Due to island growth, domain boundaries form upon coalescence of the islands. The island growth enables partial relaxation of the misfit strain. X-ray resonant magnetic reflectometry reveals that only the very first monolayers of Fe_3O_4 at the interface exhibit a reduced magnetization, presumably related to the presence of the ZnO substrate.

DF 9.67 Tue 12:15 Poster A

Spin Injection and Spin Transport in Zinc Oxide — •Matthias Althammer, Eva-Maria Karrer-Müller, Sebastian T. B. Goennenwein, Matthias Opel, and Rudolf Gross — Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching

The wide bandgap semiconductor zinc oxide is interesting for semiconductor spintronics because of its small spin-orbit coupling implying a large spin coherence length. We investigate the injection, transport, and detection of spin-polarized charge carriers in ZnO utilizing all-electrical, vertical spin valve devices with ferromagnetic electrodes. Using pulsed laser deposition and electron-beam evaporation, we fabricated epitaxial multilayers of TiN/Co/ZnO/Ni/Au on (0001)-oriented Al_2O_3 substrates with different thicknesses of the ZnO spacer layer ranging from 5 nm to 100 nm. The multilayers were patterned into vertical mesa structures with junction areas between 100 μm^2 and 400 μm^2. Magnetotransport measurements show a clear spin valve behavior. The switching fields correspond to the coercive fields of the ferromagnetic layers as determined by SQUID magnetometry. For a ZnO thickness of 15 nm, the magnetoresistance (MR) increases from 0.8% at 200 K to 8.5% at 1.8 K. We analyze the maximum MR at low temperatures as a function of the ZnO thickness in the framework of a two spin channel model with a spin-dependent interface resistance and obtain a spin drift length for ZnO of 14.3 nm.

This work was supported by the Deutsche Forschungsgemeinschaft via SPP 1285 (project no. GR 1132/14).

DF 9.68 Tue 12:15 Poster A

Spindynamics of microstructured permalloy systems — •Sven Stienen[1], Ralf Meckenstock[1], Jürgen Lindner[1], Nathalie Reckers[1], Kai Wagner[1], Florian Römer[1], Zheng Duan[2], and Michael Farle[1] — [1]Universität Duisburg-Essen, Fakultät für Physik and CeNIDE, Lotharstraße 1, 47057 Duisburg — [2]University of California, Department of Physics and Astronomy, Irvine, USA

We model a ferromagnetic resonance (FMR) measurement by micromagnetic simulations using the 3D Object Orientated Micromagnetic Framework (OOMMF) code to investigate spinwave modes in permalloy (Py) microstripes. Dispersion relations (3-12GHz) were calculated with different directions (0°/90°) of the external magnetic field (0-400mT) applied in the sample plane. The major magnetic anisotropy in the Py-stripe is the demagnetisation field. The simulations allow the visualization and identification of the excitations in the time and space domain. Quasi uniform, edge and not-aligned modes are observed. The simulations were compared with the FMR results obtained by anisotropic magneto resistance[1]. The position and shape of all modes can be explained by specific aspects of the demagnetisation field and are in qualitativly good agreement with simulations. This work has been supported by the Deutsche Forschungsgemeinschaft (DFG) via SFB 491.

[1]A. Banholzer et al, Nanotechnology, 22,(2011) 295713

DF 9.69 Tue 12:15 Poster A

Imaging of magnetisation dynamics of coupled vortices in trilayer systems — •Anja Banholzer[1], Sebastian Wintz[1], Christopher Bunce[1], Thomas Strache[1], Michael Körner[1], Arthur Erbe[1], Aleksandr Puzic[2], Jörg Raabe[2], Christoph Quitmann[2], Kilian Lenz[1], and Jürgen Fassbender[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Paul Scherrer Institut, 5232 Villigen, Switzerland

Magnetic vortices recently gained interest as potential storage media. Different control methods are used to manipulate the vortex states. We now use scanning transmission x-ray microscopy (STXM) to image the magnetic configurations within the different layers of a Co/Cu/NiFe trilayer system. The dominant coupling mechanisms here are the magneto-dipolar interaction and interlayer exchange coupling. The corresponding magnetization configurations under a static magnetic field, as well as ac magnetic fields are investigated. The emerging motion of the core is tunable by the amplitude and frequency of the field. The interactions of the two cores and their individual resonance frequencies are studied. This implies a corresponding resistance change of different configurations at different magnetic fields and currents as well as the displacement of the core.

DF 9.70 Tue 12:15 Poster A

Oersted field contribution on the magnetic vortex core dynamics probed by homodyne detection — •June-Seo Kim[1,5], Martin Stärk[1], Mathias Kläui[1,5], Florian Kronast[2], Roland Mattheis[3], Christian Ulysse[4], and Giancarlo Faini[4] —

[1]Fachbereich Physik, Universität Konstanz, Universitätsstr. 10, D-78457 Konstanz, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [3]Institut für Photonische Technologien e.V., Jena, Germany — [4]Phynano Team, Laboratoire de Photonique et de Nanostructures, CNRS, Marcoussis, France — [5]Institut für Physik, Johanes Gutenberg-Universität Mainz, D-55099, Mainz, Germany

When injecting spin-polarized currents into magnetic discs, both spin torque and Oersted fields can manipulate magnetic vortex structures. The Oersted field contribution due to the inhomogeneous current distribution in the magnetic vortex core structure is experimentally determined by using a homodyne detection scheme. We find that the amplitude of the vortex core gyration increases for vortices located close to the current injection contacts due to the enhancement of the Oersted field contribution. From systematic phase measurements as a function of microwave frequency, two remarkable phenomena are observed: (i) the trajectory of the vortex core gyration is distorted by the interaction with the disc edge leading to non-linear oscillations (ii) the interplay between spin torque and Oersted field depends sensitively on the exact vortex core position.

DF 9.71 Tue 12:15 Poster A

Ultrafast, layer-selective dynamics of interlayer exchange-coupled Fe-Ru-Ni-trilayers — •Dennis Rudolf[1], Patrik Grychtol[1], Roman Adam[1], Bastian Heller[1], Moritz Plötzing[1], Christian Weier[1], Claus M. Schneider[1], Chan La-O-Vorakiat[2], Emrah Turgut[2], Henry C. Kapteyn[2], Margaret M. Murnane[2], Stefan Mathias[3], Martin Aeschlimann[3], Justin M. Shaw[4], Hans Nembach[4], and Thomas J. Silva[4] — [1]Peter Grünberg Institut, PGI-6, Research Center Jülich, 52425, Jülich, Germany — [2]Department of Physics and JILA, University of Colorado, Boulder, Colorado 80309-0440, USA — [3]University of Kaiserslautern and Research Center OPTIMAS, 66606, Kaiserslautern, Germany — [4]Electromagnetics Division, National Institute of Standards and Technology, Boulder, Colorado, 80305-3328, USA

Using ultrafast light pulses of laser-generated high harmonics between 20 eV and 70 eV, we investigated static and dynamic properties of interlayer exchange-coupled thin Fe-Ru-Ni-trilayers with varying Ru thickness. In the static case we observed layer-selective switching of Fe- and Ni-layers. We studied the magnetization dynamics on the fs-timescale using a pump-probe technique with 1,5 eV-pump and high harmonics-probe and observed layer-selective dynamics of Fe- and Ni-layers at the M absorpion edges (54 eV for Fe and 66 eV for Ni). A comparison of the demagnetization times for parallel and antiparallel magnetization alignment of the Fe- and Ni-layers provides insight into the role of exchange interaction and spin transport in femtomagnetism.

DF 9.72 Tue 12:15 Poster A

Element-resolved Ultrafast Spin Dynamics in Multi-component Ferromagnets and Ferrimagnets — •Andrea Eschenlohr[1], Ilie Radu[1,2], Christian Stamm[1], Kadir Vahaplar[2], Torsten Kachel[1], Niko Pontius[1], Rolf Mitzner[1], Karsten Holldack[1], Alexander Föhlisch[1], Florin Radu[1], Richard F. L. Evans[3], Thomas A. Ostler[3], Johan Mentink[2], Roy W. Chantrell[3], Arata Tsukamoto[4,5], Akiyoshi Itoh[4], Andrei Kirilyuk[2], Alexey V. Kimel[2], and Theo Rasing[2] — [1]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Germany — [2]Radboud University Nijmegen, The Netherlands — [3]University of York, UK — [4]Nihon University, Chiba, Japan — [5]Japan Science and Technology Agency, Saitama, Japan

With 100 fs soft x-ray pulses generated by the Femtoslicing facility at the BESSY II storage ring we measure element-resolved transient x-ray magnetic circular dichroism in ferromagnetic NiFe alloys, as well as ferrimagnetic GdFeCo alloy after laser excitation. We find time constants of demagnetization that are not only different for each magnetic sublattice in our alloy samples, but also different from the time constants found for respective pure element samples. Supported by phenomenological considerations and atomistic simulations we conclude that sub-picosecond magnetization dynamics is sensitive to both the magnetic moment and exchange interaction between the sublattices in multi-component magnets.

DF 9.73 Tue 12:15 Poster A

Gyration of magnetic vortices in anharmonic potentials — •Christian Adolff, Michael Martens, Thomas Kamionka, Ulrich Merkt, and Guido Meier — Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg, Jungiustr. 11, 20355 Hamburg, Germany

Magnetic vortices inherently form in soft ferromagnetic thin-film elements. They can be described as quasiparticles in confining potentials with eigenfrequencies in the sub-gigahertz range [1, 2]. We investigate the excitation of magnetic vortices in permalloy squares with side lengths of up to five micrometers. Strongly excited vortex cores move near to the edges of the squares where significant deviations from a parabolic potential occur. Analyzing the eigenfrequency of the vortex for different geometries, i.e. side lengths and thicknesses, gives insight into isotropic and anisotropic terms of the potential. These are studied by means of ferromagnetic resonance spectroscopy, micromagnetic simulations and analytical calculations.

[1] A. Thiele, J. Appl. Phys. 45, 377 (1974)
[2] B. Krüger et al., Phys. Rev. B 76, 224426 (2007)

DF 9.74 Tue 12:15 Poster A

Magnetization dynamics in Ni on the picosecond timescale — •Martin Lüttich[1], Jakob Walowski[1], Andreas Mann[1], Markus Münzenberg[1], Unai Atxitia[2], and Oksana Chubykalo-Fesenko[2] — [1]I. Physikalisches Institut, Universität Göttingen — [2]Instituto de Ciencia de Materiales de Madrid

Magnetization dynamics of polycrystalline nickel films are measured using the all-optical pump-probe technique for various pump pulse fluences. The parallel treatment of photons, electrons, phonons and magnetic correlations of the system amounts a challenge to the microscopic theoretical description. At the same time different length and time scales are involved.

We investigate the influence of hot electrons on the relative demagnetization. Performing the experiment for different pump fluences, we measure a higher relative demagnetization at higher fluences. These results are compared to simulations with the Landau-Lifshitz-Bloch equation, which is based on a thermal model, and featured by the consideration of two electron temperature dependent relaxation times $\tau_\perp$ and $\tau_{||}$. The electron temperature needed as input for the simulations is extracted from experiments.

DF 9.75 Tue 12:15 Poster A

Ultrafast Demagnetization Dynamics in $Ni_{1-x}Pd_x$ alloys — •Moritz Plötzing[1], Patrik Grychtol[1], Roman Adam[1], Claus M. Schneider[1], Hans Nembach[2], Justin Shaw[2], Tom Silva[2], Oliver Schmitt[3], Daniel Steil[3], Mirko Cinchetti[3], and Martin Aeschlimann[3] — [1]Peter Grünberg Institut, PGI-6, Research Center Jülich, 52425, Jülich, Germany — [2]Electromagnetics Division, National Institute of Standards and Technology, Boulder, Colorado 80305-3328, USA — [3]University of Kaiserslautern and Research Center OPTIMAS, 67663, Kaiserslautern, Germany

In the presented work, we investigated alloys of Ni and Pd with varying mixing ratios focusing on the magnetization dynamics on different timescales. For this purpose, we characterized the samples using a vibrating sample magnetometer and ferromagnetic resonance in order to determine the Curie temperature T_C and the picosecond dynamics, respectively. The latter is described by the Gilbert damping parameter α. Both quantities depend strongly on the stoichiometry and can be tuned very precisely over a wide range by changing the Pd concentration. Additionally, we carried out a thorough investigation of the laser-induced demagnetization time τ_M on the femtosecond timescale employing a time-resolved MOKE setup. According to the theoretical model published in [1], the dynamics on both timescales is related and the proportionality is mainly defined by T_C. Using the measured values for α and τ_M, we study the applicability of the theory for a ferromagnetic d-alloy and consequently the underlying fundamental processes.

[1] Koopmans et al., Phys. Rev. Lett. 95, 267207 (2005)

DF 9.76 Tue 12:15 Poster A

Ultrafast magnetization dynamics of FePt:Cu — •Daniel Steil[1], Sabine Alebrand[1], Oliver Schmitt[1], Mirko Cinchetti[1], Martin Aeschlimann[1], Fabian Ganss[2], Christoph Brombacher[2], and Manfred Albrecht[2] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Institute of Physics, Chemnitz University of Chemnitz, 09107 Chemnitz, Germany

$L1_0$ ordered FePt compounds with out of plane anisotropy are one future candidate as a storage layer for the next generation of hard disc drives, due to their very high anisotropy energy. As these compounds typically have very high coercivity, they are best used in combination

with heat assisted recording (HAMR) [1]. We have studied the demagnetization dynamics in the alloy system FePt:Cu following impulsive laser excitation. In particular we also investigated the helicity dependence of the magnetization dynamics. By adding copper to FePt it is possible to tune anisotropy and Curie temperature, which allows to study the influence of both parameters on magnetization dynamics. We find a fast and strong demagnetization for all sample compositions, leading to a long lasting multidomain state for high enough excitation fluences in remanence. Additionally we observe a small influence of light helicity on the magnetization dynamics for at least one of the samples, whose origin will be discussed.

Funding by the EU within the FP7 project UltraMagnetron is kindly acknowledged.

[1] D. Weller et al., Annu. Rev. Mater. Sci. 30, 611-644 (2000)

DF 9.77 Tue 12:15 Poster A

Angular and Temperature dependent Ferromagnetic Resonance (FMR) measurements on FeRh thin films — •Eduardo Mancini, Federico Pressacco, Markus Härtinger, Georg Woltersdorf, and Christian Back — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Regensburg, Deutschland

We report the results of FMR investigations performed on $Fe_{0.5}Rh_{0.5}$(30 nm)/MgO below and above the critical temperature (around 400 K) at which the magnetic order changes from the antiferromagnetic- to the ferromagnetic phase. From these measurements we extract the amplitude, the position and the linewidth of the resonance line. For the amplitude the heating and cooling branches display the hysterestic behavior which is expected for this material with a difference in their critical temperatures of about 10 K. In the ferromagnetic phase (T=450 K), we observe an easy plane anisotropy for the magnetization from the analysis of the resonance position as a function of the external field orientation. From the linewidth of the resonance we extract the damping of the magnetization and discuss its temperature dependence in the neighborhood of the critical temperature.

DF 9.78 Tue 12:15 Poster A

Time-resolved Scanning-Kerr-Microscope on Rolled-Up-Ferromagnetic-Microstructures — •Daniel Mellem, Sebastian Mansfeld, Jan-Niklas Toedt, Felix Balhorn, Lennard Moldenhauer, Wolfgang Hansen, Detlef Heitmann, and Stefan Mendach — Institut für Angewandte Physik, Jungiusstr. 11, D-20355 Hamburg

Our time-resolved Scanning-Kerr-Microscope (TR-SKM) [1] is used to directly image propagating spin waves. We introduce the working principle of our Microscope and present first measurements of spin waves in rolled-up ferromagnetic structures, which were recently introduced as a novel type of flexible spin wave resonator by our group [2].

We gratefully acknowledge support by the DFG via SFB668 and GrK 1286.

[1] S. Mansfeld et al., Physical Review Letters, in press (2011)
[2] F. Balhorn et al. PRL 104, 037205, 2010

DF 9.79 Tue 12:15 Poster A

Spin-Wave Confinement in Rolled-Up Permalloy Nano-Stripes in Various Magnetization Configurations — •Lennart Moldenhauer, Felix Balhorn, Daniel Mellem, Sebastian Mansfeld, Wolfgang Hansen, Detlef Heitmann, and Stefan Mendach — Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg, Jungiustr. 11, 20355 Hamburg, Germany

A variety of planar systems consisting of magnetic nano- and microstripes have recently been investigated in terms of their magnetodynamic behavior [1]. Using the concept of self-rolling strained layers [2] we realized rolled-up Permalloy (Py) stripes.

We studied the spin-wave behavior in these three dimensional self-organized structures in different magnetic configurations and for varying geometrical stripe parameters via broadband microwave absorption spectroscopy. We discuss our measurements in terms of azimuthal and axial spin-wave confinement. We compare our results to previous experiments on planar stripes and rolled-up films [3].

[1] J. Topp et al., PRB **78**, 024431 (2008); [2] V. Y. Prinz et al., Physica E **6**, 828-831 (2000); [3] F. Balhorn et al., PRL **104**, 037205 (2010)

DF 9.80 Tue 12:15 Poster A

Ultrafast magnetic dynamics in EuTe thin films — •Niko Pontius[1], Christoph Trabant[1,2], Enrico Schierle[1], Eugen Weschke[1], Torsten Kachel[1], Christian Schüssler-Langeheine[1], Rolf Mitzner[1], Günther Springholz[3], and Karsten Holldack[1] — [1]Helmholtz-Zentrum Berlin — [2]II. Physikalisches Institut, Universität zu Köln — [3]Institut für Halbleiterphysik, Johannes Kepler Universität, Linz, Austria

Ultrafast control of magnetic materials and structures are a key prerequisite for developing advanced magnetic storage devices with increased speed and decreased dimensions. To this end, investigations of confined magnetic structures behaviour apart from equilibrium with sufficient spatial and temporal resolution under as defined conditions as possible are essential.

Here we investigate the fs temporal non-equilibrium evolution of the antiferromagnetic (AFM) order in EuTe thin films through resonant soft x-ray diffraction after laser excitation. Momentum resolved scans across the Bragg reflection provide information on the thin film magnetic profile evolution during the ultrafast quenching and recovery of the AFM order. They reveal that the magnetic profile is modified in a completely different way than for elevated temperatures in thermal equilibrium. Since the AFM structure of EuTe sensitively depends on the ionic distances, this study also provides new information on the interplay between structural and magnetic degrees of freedom. The measurements were performed at the FemtoSPEX facility at the HZB.

DF 9.81 Tue 12:15 Poster A

Temperature dependence of the magnon dispersion relation in low-dimensional transition-metal systems: A first-principles investigation — •Waldemar Töws and Gustavo M. Pastor — Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel

The influence of Stoner excitations on the spin-wave spectrum of one- and two-dimensional 3d transition metals has been investigated. The physical situations represented by the Stoner excitations correspond to extreme nonequilibrium states, which can be induced by strong ultrashort laser pulses. In this work we quantify to what extent an important increase of the electronic temperature T_e describing Stoner excitations affects the stability of magnetism within the metal. For this purpose, we perform numerical calculations in the framework of *ab initio* density-functional theory with a generalized gradient approximation to the exchange and correlation energy. The free energy of frozen-magnon states as a function of spin-wave vector q and T_e have been systematically studied for V, Fe, Co and Ni wires and monolayers with various nearest-neighbor distances. First of all, we demonstrate that the local magnetic moments are extremely stable even at temperatures T_e much larger than the Curie temperature T_C. The T_e-dependence of the magnetic couplings between the local moments is quantified by fitting the effective exchange couplings J_{ij} to the free-energy dispersion relation in the framework of a classical spin model. One actually finds that electronic temperatures T_e well above T_C are needed to change the nature of the magnetic order within the metal. The consequences for the theory of laser-induced magnetization dynamics are discussed.

DF 9.82 Tue 12:15 Poster A

Time Resolved Scanning Kerr Microscopy of Structures in thin ferromagnetic Films — •Jan-Niklas Toedt, Sebastian Mansfeld, Jesco Topp, Kim Martens, Daniel Mellem, Wolfgang Hansen, Detlef Heitman, and Stefan Mendach — Institute of Applied Physics, University of Hamburg

We study the behavior of planar Damon-Eshbach spin-waves in thin structured ferromagnetic films utilizing time resolved scanning Kerr microscopy (TR-SKM) [1]. We have investigated spin waves incident on a range of structures including gratings, double slits and modulated films. We show that the underlying physics can be explained by the anisotropy of the dispersion relation leading, e.g., to sub wavelength imaging [2, 3].

We gratefully acknowledge support by the DFG via SFB 668, SFB 508, GrK 1286, and by the City of Hamburg via the Cluster of Excellence Nano-Spintronics.

[1] Freeman et al., Journal of Applied Physics **79**, 5898 (1996); [2] Liu et al., Science **315**, 1686 (2007); [3] Mansfeld et al., Physical Review Letters, in press (2011) - arXiv:1108.5883v1

DF 9.83 Tue 12:15 Poster A

Field-induced magnetization dynamics in dot patterned CoB/Pt multilayer structures — •F. Büttner[1,2,3,4], C. Moutafis[2,3], A. Bisig[1,2,3,6], C.M. Günter[4], J. Geilhufe[5], M.

Schneider[4], C. v. Korff Schmiesing[4], M. Hantschmann[4], M. Riemeier[4], J. Mohanty[4], S. Schaffert[4], J. Franken[7], R. Lavrijsen[7], H. J. M. Swagten[7], H. Stoll[8], M. Weigand[5,8], M. Kläui[1,2,3,6], and S. Eisebitt[4,5] — [1]Uni Mainz, 55128 Mainz, Germany — [2]PSI, 5232 Villigen, Switzerland — [3]EPF Lausanne, 1015 Lausanne, Switzerland — [4]TU Berlin, 10623 Berlin, Germany — [5]HZB, 12489 Berlin, Germany — [6]Uni Konstanz, 78457 Konstanz, Germany — [7]TU Eindhoven, 5612 AZ Eindhoven, Netherlands — [8]MPI für Metallforschung, 70569 Stuttgart, Germany

The controlled movement of nanometer sized magnetic domains on the (sub-) nanosecond time scale is of key importance for the development of new magnetic devices in storage and computing technology. While magnetization dynamics in in-plane magnetized materials has been intensely studied, domain sizes are too large for most state-of-the-art applications. In out-of-plane materials, however, we find narrow domains and domain walls, but these are much more sensitive to local pinning, thus making controlled displacements extremely challenging. We present here high resolution magnetic images of low pinning CoB/Pt multilayer structures and demonstrate the suitability of this material for controlled and reproducible field-induced dynamics of the magnetic domains on the nanosecond time scale.

DF 9.84 Tue 12:15 Poster A

Spin-wave tunneling through a mechanical gap in microstructured $Ni_{81}Fe_{19}$-stripes — •Thomas Langner[1], Björn Obry[1], Philipp Pirro[1], Thomas Brächer[1,2], Katrin Vogt[1,2], Britta Leven[1], and Burkard Hillebrands[1] — [1]TU Kaiserslautern, Fachbereich Physik and Forschungszentrum OPTIMAS, Erwin-Schrödinger-Str. 56, 67663 Kaiserslautern — [2]Graduate School Materials Science in Mainz, Gottlieb-Daimler-Straße 47, 67663 Kaiserslautern

The manipulation of the propagation properties of spin waves is of high importance to develop systems that can transport information using the spin wave as information carrier. One way to manipulate these properties is the use of magnetic tunnel barriers. We investigated the tunneling of spin waves through a mechanical gap in microstructured stripes made of $Ni_{81}Fe_{19}$. The focus of this work is on the investigation of the transmission of spin waves with varying wavelengths through a tunnel barrier with respect to the position of the gap. It is shown that quantization effects play an important role in the transmission behavior of tunneling spin waves in microscaled systems. The region between the excitation antenna and the gap acts as a spin-wave resonator. It has a large influence not only on the excitation properties but also on the transmission characteristics. We present Brillouin light scattering microscopy measurements revealing a strong influence of pinning effects of standing spin-wave modes inside this resonator on the tunneling efficiency.

DF 9.85 Tue 12:15 Poster A

Spin-wave logic elements based on ferromagnetic microstructures — •Jan Westermann[1], Philipp Pirro[1], Thomas Brächer[1,2], Björn Obry[1], Katrin Vogt[1,2], Roland Neb[1], Britta Leven[1], and Burkard Hillebrands[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Graduate School Material Science in Mainz, 67663 Kaiserslautern, Germany

The investigation of propagating spin waves in micron-sized metallic ferromagnetic structures is subject of different experimental studies due to their potential application in spin-wave logic devices. Using the amplitude and the phase of the spin waves, these devices may provide outstanding performance, especially when operated with multiple frequencies.

We present micro-magnetic simulations focused on the feasibility of micro-structured spin-wave logic elements as well as an experimental investigation of short wavelength spin waves. The controlled excitation and the propagation of those spin waves is essential for efficiently working spin-wave logic elements. To analyze the excitation spectrum we use phase resolved Brillouin Light Scattering Microscopy to observe the spin waves in single micro-structures. For these experiments, we excite spin waves using different kinds of microwave antennas which show geometry dependent excitation spectra. Our experimental and numeric investigations show that magnetic micro-structures are promising candidates for wave-logic based elements. Financial support by Carl-Zeiss-Foundation, MAINZ and DFG is gratefully acknowledged.

DF 9.86 Tue 12:15 Poster A

Quantitative modeling of elastically driven ferromagnetic resonance — •Matthias Pernpeintner[1], Mathias Weiler[1], Lukas Dreher[2], Hans Huebl[1], Christian Heeg[1], Rudolf Gross[1], Martin S. Brandt[2], and Sebastian T. B. Goennenwein[1] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Walter Schottky Institut, Technische Universität München, 85748 Garching, Germany

In conventional ferromagnetic resonance (FMR) experiments, an external radio frequency magnetic field drives the magnetization precession. Recently, it has been shown that FMR can be excited all elastically by means of coherent phonons [1]. In this acoustically driven FMR, the magnetoelastic coupling of surface acoustic waves (SAW) in the GHz frequency range with a thin ferromagnetic film is exploited.

Here we show that acoustically driven FMR can be phenomenologically modeled using a modified Landau-Lifshitz-Gilbert approach in which the SAW induces an internal, virtual magnetic driving field. In a quantitative analysis, the magnetization dynamics are calculated as a function of external magnetic field magnitude and orientation. Full quantitative agreement of this simulation and SAW transmission experiments performed in a $Ni/LiNbO_3$ hybrid device is shown, using a set of parameters consistent with literature data.

This opens the path for further experimental studies of resonant magnon-phonon coupling and acoustic spin current generation using elastically driven magnetization dynamics.

[1] M. Weiler *et al.*, Phys. Rev. Lett. **106**, 117601 (2011).

DF 9.87 Tue 12:15 Poster A

Microscopic magnetic structuring of spin-wave wave- guides by ion implantation in a $Ni_{81}Fe_{19}$ layer — •Thomas Meyer[1], Björn Obry[1], Philipp Pirro[1], Thomas Brächer[1,2], Roland Neb[1], Julia Osten[3], Thomas Strache[3], Jürgen Fassbender[3], and Burkard Hillebrands[1] — [1]FB Physik and Landesforschungszentrum OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Graduate School Materials Science in Mainz, 67663 Kaiserslautern, Germany — [3]Institut für Ionenstrahlphysik und Materialforschung, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Ion implantation of ferromagnetic films has proven to be a promising tool for the fabrication of fully planar samples with a microscopic magnetic substructure. A waveguide-like propagation of spin waves in a $Ni_{81}Fe_{19}$ film which was locally patterned by ion implatation could be observed. The investigations have been performed using Brillouin light scattering microscopy on samples patterned with varying ion fluences. Further investigations on the coupling behaviour of two parallel stripes in this fully planar structures have been performed. The presented fabrication technique of spin-wave waveguides provides much lower stray fields and better heat conduction. Especially the latter is a matter of interest when the objects are exposed to intense microwave fields (excitation of spin waves) or investigated by laser spectroscopy like Brillouin light scattering. Financial support by the DFG (GRK 792) is gratefully acknowledged.

DF 9.88 Tue 12:15 Poster A

Thermally modulated ferromagnetic resonance in planar microresonator — •Puchong Kijamnajsuk[1,2], Christian Schöppner[1], Sven Stienen[1], Detlef Spoddig[1], Ralf Meckenstock[1], and Josef Pelzl[2] — [1]Universität Duisburg-Essen, Standort Duisburg, Institut für Physik und CeNIDE, AG Farle, Lotharstr. 1, 47048 Duisburg — [2]Institute of Experimental Physics, Ruhr University Bochum

A novel approach based on the combination of two scanning thermal near field techniques: the thermally modulated ferromagnetic resonance (FMR) by the probe of a scanning thermal wave microscope and the 3ω-signal from the same thermal probe. The simultaneous detection of the thermally modulated microwave absorption and of the 3ω-response of the nano-probe offers a means to control the thermal contact between probe and sample. To enhance the sensitivity of the FMR detection for the single 30nm x 30nm x 30nm ferromagnetic Heusler alloy $Ni_{45}Mn_{37}In_{13}Co_5$, we have designed a microresonator setup. The constant amplitude microwave field is generated inside the resonator at the position of the sample at a fixed frequency 14GHz. To observe the FMR we apply the fixed external magnetic field and modulate the sample temperature by joule heating from the probe. With the microresonator we demonstrate the detection of FMR of a single nano-sized cube.

DF 9.89 Tue 12:15 Poster A

Broadband Electron Spin Resonance Experiments using su-

perconducting Coplanar Waveguides — •Conrad Clauss[1], Daniel Bothner[2], Lapo Bogani[1], Marc Scheffler[1], Dieter Koelle[2], Reinhold Kleiner[2], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, D-70550 Stuttgart, Germany — [2]Physikalisches Institut - Experimentalphysik II and Center for Collective Quantum Phenomena in LISA+, Universität Tübingen, D-72076 Tübingen, Germany

In recent years superconducting coplanar devices operating at microwave/GHz frequencies are employed in more and more experimental studies.

Here, we present electron spin resonance (ESR) experiments using a superconducting coplanar waveguide to provide the RF field to drive the spin flips. In contrast to conventional ESR studies this allows broadband frequency as well as magnetic field swept observation of the spin resonance.

We show experimental data of the spin resonance of the organic radical NitPhoMe (2-(4'-methoxyphenyl)-4,4,5,5-tetra-methylimidazoline-1-oxyl-3-oxide) for frequencies in the range of 1 GHz to 40 GHz and corresponding magnetic fields up to 1.4 T (for g=2). In addition we show the temperature dependence of the ESR signals for temperatures up to 30 K, which is well above the critical temperature of the niobium superconductor.

DF 9.90 Tue 12:15 Poster A

Studying magnetic nanostructures and the local magnetic induction of bulk samples by micro-Hall magnetometry — •Merlin Pohlit[1], Pintu Das[1], Adham Amyan[1], Yuzo Ohno[2], Hideo Ohno[2], and Jens Müller[1] — [1]Physikalisches Institut, Goethe-Universität, Frankfurt (M), Germany — [2]Laboratory for Nanoelectronics and Spintronics, Tohoku University, Sendai, Japan

Hall magnetometers based on high-mobility two-dimensional-electron systems in GaAs/AlGaAs heterostructures are powerful tools for studying individual magnetic structures on the micro- and nanoscale [1]. In particular, the devices can be used in a wide temperature and magnetic field range. Besides the possibility to position magnetic structures directly on top of the lithographically defined Hall crosses, bulk magnetic and superconducting samples may be placed on the magnetometers for local magnetic induction measurements. Here, a series of adjacent Hall crosses allows for spatially-resolved measurements with micron-size resolution. The versatility of the devices can be demonstrated by different measuring techniques including eight-terminal Hall gradiometry, magnetic flux noise measurements and the use as susceptometers. We discuss various examples for these methods, e.g. on the ferromagnetic semimetal EuB_6, where two consecutive transitions occur at 15.5K and 12.6K.These are related to electronic and magnetic phase separation and bulk magnetic ordering, but the details are not yet fully understood. We perform stray field calculations in order to simulate our results and find good agreement with the experimental data. [1] P. Das et al., APL 97, 042507 (2010)

DF 10: High- and low-k-dielectrics (jointly with DS)

Time: Wednesday 9:30–11:30 Location: EB 407

DF 10.1 Wed 9:30 EB 407

High dielectric constants due to charge order induced electrical heterogeneity — •Stephan Krohns[1], Pit Sippel[1], Holger Kirchhain[1], Stefan Riegg[1], Peter Lunkenheimer[1], Armin Reller[2], and Alois Loidl[1] — [1]Experimental Physics V, University of Augsburg — [2]Resource Strategy, University of Augsburg

One of the most imminent challenges of modern materials science is the development of new materials with less critical elements that have comparable or better functionalities than those currently used. We illustrate an interdisciplinary approach by applying it to the prototypical example of materials with extremely high dielectric constant to validate the innovative potential in a very early stage of research.[1]

Not only the validation of the economic and technical potential of high dielectric constant materials are in the focus of interest, but also the mechanisms generating this dielectric phenomena. Most of the materials exhibiting those effects, among them numerous transition-metal oxides[2], have complex ground states emerging from strong electronic correlations. $La_{15/8}Sr_{1/8}NiO_4$ for example shows a very high dielectric constant up to gigahertz frequencies at room temperature and it seems that charge order induced electrical heterogeneity can be the origin. To scrutinize that, we also thoroughly investigate the structural, magnetic and dielectric properties of various isostructural $La_{2-x}(Ba,Ca,Sr)_xNiO_4$ compounds especially emphasizing the contribution of electronic phase separation to the permittivity.

[1] S. Krohns *et al.*, Nat. Mat. **10**, 899 (2011). [2] P. Lunkenheimer *et al.*, Eur. Phys. J. Special Topics **180**, 61 (2010).

DF 10.2 Wed 9:50 EB 407

Bilayer gate dielectric stacks of cerium oxide and titanium oxide for nanoelectronics — •Meng Meng Vanessa Chong[1,2], Kam Chew Leong[2], Pooi See Lee[1], and Iing Yoong Alfred Tok[1] — [1]School of Materials Science and Engineering, Nanyang Technological University, Block N4.1, Nanyang Avenue, Singapore 639798 — [2]Global Foundries Singapore Pte. Ltd., Singapore 528830

Numerous materials systems are under consideration as potential replacements for SiO2 as the gate oxide material for sub-0.1 micron CMOS technology. Many properties have to be considered in selecting a suitable material because of emerging issues with high-k technology development. Though, many dielectrics appear favorable in some of these areas, but very few materials are promising with respect to all the required properties.

This work focuses on the rare earth oxide - CeO2 as alternative dielectric as it has small lattice mismatch with Si and high k-values. This study also shows the integration of a high-k passivation layer (TiO2) to suppress the formation of undesirable interfacial layer. Physical characterizations are done to determine the stoichiometry, surface roughness and interface quality.

In addition, temperature dependent measurements are done to identify the different conduction mechanisms such as Poole-Frenkel emission. Identification of various leakage constituent is important for estimation and reduction of leakage power. Furthermore, in-depth electrical analysis helps to determine the quality of the film and dielectric interface.

DF 10.3 Wed 10:10 EB 407

High quality REO thin films from wet chemical deposition — •Maraike Ahlf[1,2], Meng Meng Vanessa Chong[2,3], Mathias Wickleder[1], Alfred Iing Yoong Tok[2], Pooi See Lee[2], and Katharina Al-Shamery[1] — [1]University of Oldenburg, IRAC, Germany — [2]Nanyang Technological University, MSE, Singapore, Singapore — [3]Global Foundries Ltd., Singapore

The aggressive scaling in microelectronics leads to the need of new high performance thin film materials as gate oxides in MOS devices. High leakage currents suffered for conventionally used SiO_2 when scaling down to sub 22 nm requires alternative high κ dielectrics. REOs are potential candidates to replace SiO_2 due to their ecellent electrical properties. This necessitates the synthesis of new RE precursors and deposition methods to achieve impurity free films, since conventionally used techniques suffer from problems such as C impurities from the organic precursors used and formation of interfacial layers or byproducts due to high process temperatures. Results of an unconventional, low temperature, patented, wet chemical approach which is easy to realize and integrate into device production to deposit Nd_2O_3 ultra thin, high quality gate stacks will be presented. The constitution and annealing dependent crystallization behavior on Si and the deposition mechanism of inorganic designer RE-precursors has been investigated with XPS, XRD, AFM and HRTEM. CV and IV measurements show κ values as twice as high and leakage currents down to 10 orders of magnitude lower than conventionally SiO_2. Various current conduction mechanisms can be understood from varying temperature measurements.

DF 10.4 Wed 10:30 EB 407

Epitaxial growth of $Ba_{0.6}Sr_{0.4}TiO_3$ on highly conductive $SrMoO_3$ thin films by Pulsed Laser Deposition — •Aldin Radetinac, Philipp Komissinskiy, and Lambert Alff — Institut für Materialwissenschaften, Technische Universität Darmstadt, Petersenstraße 23, 64287 Darmstadt, Germany

High-quality thin films and heterostructures of dielectric and conducting oxides are necessary for realization of all-oxide tunable capacitors.

Here we present epitaxial $Ba_{0.6}Sr_{0.4}TiO_3/SrMoO_3$ (BST/SMO) heterostructures grown by Pulsed Laser Deposition (PLD) on single crystal $SrTiO_3$ (100) and $GdScO_3$ (110) substrates. 80 nm thick highly conducting (001) SMO films with a resistivity below 100 $\mu\Omega$cm are deposited in argon atmosphere at $5x10^{-4}$ Torr [1]. A 5 nm thick initial epitaxial BST buffer layer is grown at low oxygen pressure of 10^{-5} Torr and flow of 0.7 sccm. The buffer layer prevents oxidation of the SMO film to $SrMoO_4$ and allows further deposition of the fully oxidized paraelectric BST at oxygen pressure of $5x10^{-4}$ Torr and 0.9 sccm flow. To our knowledge this study shows for the first time how metastable materials like SMO can be incorporated in oxide electronic devices. The work is supported by the GRK 1037 (TICMO) project of the DFG.

[1] A. Radetinac, K. S. Takahashi, L. Alff, M. Kawasaki and Y. Tokura, Appl Phys Express 3 (7) (2010)

DF 10.5 Wed 10:50 EB 407

***P*-type conductivity in oxygen deficient HfO_{2-x} thin films grown by Reactive Molecular Beam Epitaxy** — •Erwin Hildebrandt[1], Jose Kurian[1], Mathis Müller[1], Thomas Schroeder[2], Hans-Joachim Kleebe[1], and Lambert Alff[1] — [1]Institute of Materials Science, Technische Universität Darmstadt, Germany — [2]IHP, Frankfurt(Oder), Germany

Highly oxygen deficient thin films of hafnium oxide HfO_{2-x} were grown using reactive molecular beam epitaxy on *c*-cut sapphire substrates. The oxygen content and, thus, oxygen vacancy concentration was engineered by controlled oxidation using RF-activated oxygen during growth. Hafnium oxide, a high-*k* dielectric insulator in its stoichiometric form, turns into a *p*-type semiconductor above a threshold of oxygen vacancies with up to 6 times 10^{21} charge carriers per cm^3. The introduction of oxygen vacancies reduces the optical band gap from 5.7 eV for stoichiometric HfO_2 by more than 1 eV. The absence of crystalline and/or amorphous metallic hafnium phases was proven by X-ray diffraction and a tilting series using High-Resolution Transmission Electron Microscopy. We suggest the formation of an oxygen vacancy induced *p*-type defect band within the energy gap as the origin of the observed *p*-type conductivity [1].

[1] E. Hildebrandt, J. Kurian, M. M. Müller, T. Schroeder, H.-J. Kleebe, and L. Alff, Appl. Phys. Lett. **99**, 112902 (2011).

DF 10.6 Wed 11:10 EB 407

Hydrogen Impurity in Y_2O_3: an *Ab – Initio* and a μSR perspective — •Estelina L. Silva, Apostolos Marinopoulos, Rui Vilão, and Ricardo Vieira — CEMDRX and CFC, Physics Department, University of Coimbra, P-3004-516 Coimbra, Portugal

Density functional calculations were performed for interstitial hydrogen in Y_2O_3, by employing the semi-local GGA-PBE and the hybrid HSE06 exchange-correlation functionals. It was observed that the lowest energy H^0 and H^- configurations prefer to relax in the interstitial, vacant O, sites. For these charge systems, two different geometrical configurations (interstitial vacant Y and bond O-H type) also occur as higher-energy metastable sites. In contrast, the H^+ equilibrium state was found only when a O-H bond is formed. The overall results for the formation energies, obtained by employing the two functionals are consistent, for which amphoteric behavior was found for hydrogen after considering the lowest-energy structures for each charge state. To compare results with μSR measurements, the formation energies of the metastable configurations were also evaluated. The results are consistent with the μSR data, where the co-existence of the observed diamagnetic signal is attributed to a shallow donor-like muonium and the paramagnetic signal to an acceptor-like deep muonium configuration.

For the interstitial configurations, of the neutral and negative charge systems, a defect level was found in the gap and positioned slightly above the valence band maximum, whereas for the bond O-H site, the defect level is located above the middle of the band gap, closer to the conduction band.

DF 11: Optical and nonlinear optical properties, photonic

Time: Wednesday 9:30–12:20 Location: EB 107

DF 11.1 Wed 9:30 EB 107

Dispersive properties of small polaron-based hologram recording in nominally undoped, thermally reduced $LiNbO_3$ — •Hauke Bruening and Mirco Imlau — Department of Physics, University of Osnabrück, Germany

We recently discovered a new type of hologram recording in nominally undoped, thermally reduced $LiNbO_3$ by means of a single intense ns-laser pulse ($\lambda = 532$ nm) yielding short-lived volume phase-gratings with unique features [1]: a diffraction efficiency η of more than 20% in the NIR spectral range ($\lambda = 785$ nm), a stretched-exponential relaxation behavior of the grating efficiency with a lifetime in the ms-range at room temperature, an acceleration of the decay with increasing temperature and a pronounced dependence of η on the orientation of the grating vector with respect to the polar c-axis. This type of hologram recording could be successfully modeled by taking into account an optically generated spatial modulation of small bipolarons, bound and free polarons. In this contribution, we face the unique dispersive properties of this type of hologram recording and particularly present our results for probing the gratings in the blue-green spectral range ($\lambda = 488$ nm). We show that the contribution of small bound hole polarons has to be considered as well. It can be concluded that a diffraction efficiency of about $\eta \approx 0.5 \cdot 10^{-4}$ at the telecommunication wavelength ($\lambda = 1550$ nm) can be expected.

*Financial support by the DFG (IM37/5 and INST190/137-1) and DAAD (50445542) is gratefully acknowledged.

[1] M. Imlau et al., Optics Express 19, 15322 (2011)

DF 11.2 Wed 9:50 EB 107

Quantitative examination of out-of-phase mixed holographic gratings — •Kay-Michael Voit, Hauke Bruening, and Mirco Imlau — Department of Physics, University of Osnabrück, Germany

Modern holographic applications require advanced photosensitive materials that particularly obey alterations of the complex permittivity with pronounced amplitudes of both real and imaginary parts on the sub-ps-time scale. Promising candidates such as amorphous and crystalline materials remarkably show a mutual phase-shift between phase and absorption gratings that complicates the analysis of the underlying wave-coupling mechanisms. Hence, theoretical descriptions that are simply based on Kogelnik's coupled-wave theory can not be applied, i.e., a formal approach to systematically derive the full parameter space of the gratings from diffraction efficiency measurements is missing in literature. We revised the analysis of the wave-coupling theory omitting former approximations or applying them later. As a result we derived a formal description for mixed gratings allowing for a full description of beam-coupling experiments. Both the modulations of the refractive index and the absorption coefficient as well as the phase shift between these gratings can be determined through measurements of the angular dependent diffraction efficiency around the positive and the negative Bragg angle. Our approach and results are demonstrated along a mixed grating with a most common parameter set.

*Financial support by the DFG (projects IM 37/5, INST 109/137) is gratefully acknowledged.

DF 11.3 Wed 10:10 EB 107

Surface plasmon resonance of Ag nanoclusters and refractive index changes in ion irradiated lithium niobate — •Jura Rensberg, Steffen Milz, Carsten Ronning, and Werner Wesch — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Lithium niobate ($LiNbO_3$) is one of the most important materials for integrated optics, because of its unique electro-optical and nonlinear optical properties. Ion beam synthesis plays a key role in fabricating arrays of metal nanoclusters embedded in $LiNbO_3$ particularly with regard to plasmonic applications. Major challenges of this technique are on the one hand to control the cluster size distribution and on the other hand to avoid irradiation damage of the $LiNbO_3$. Therefore we have implanted 380 keV Ag^+ ions up ton an ion fluence of $1x10^{17}$ cm^{-2} into $LiNbO_3$ at room temperature. As a consequence Ag clusters nucleated and a broad amorphous layer was produced. Isochronal rapid thermal annealing as well as isothermal annealing were performed in

the temperature range of 573 K to 1173 K, which leads to refractive index changes associated with lattice structure recovery.

In this contribution we shall report on polarization dependent optical spectroscopy of the surface plasmon resonance of silver nanoclusters embedded in $LiNbO_3$ combined with Mie theory simulations to investigate the refractive index changes upon ion irradiation and annealing.

DF 11.4 Wed 10:30 EB 107

Vergleich der optischen Materialmodifikationen von Lithiumniobat-Kristallen durch den Beschuss verschiedener schneller leichter Ionen — •Johannes Goetze, Niels L. Räth, Konrad Peithmann und Karl Maier — Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn

Lithiumniobat-Kristalle finden vielfach Anwendung in Wissenschaft und Technik, insbesondere in optischen Technologien. Methoden zur gezielten Strukturierung wichtiger Materialparamater, wie des Brechungsindex, der elektrischen Leitfähigkeit oder der ferroelektrischen Polungseigenschaften, sind daher gefragt.

Durchstrahlung der Kristalle mit hochenergetischen leichten Ionen, wie beispielsweise ^{3}He, ist eine leistungsfähige Methode zur Beeinflussung der Materialparameter. Da sie als Nebenwirkung eine parasitäre Aktivierung der Kristalle mit sich bringt, wird durch den Einsatz verschiedener Projektile (^{3}He, ^{4}He, ^{1}H, ^{2}D) untersucht, ob eine Optimierung des Prozesses möglich ist.

Der Einfluss der Projektilwahl hinsichtlich der oben genannten Bereiche soll vorgestellt werden.

10 min. break

DF 11.5 Wed 11:00 EB 107

Finding optimal starting points for quasi-particle band structures and optical properties of transparent conducting oxides. — •Martin Stankovski[1], Anna Miglio[1], David Waroquiers[1], Gabriel Antonius[2], Matteo Giantomassi[1], Michel Côté[2], Xavier Gonze[1], and Gian-Marco Rignanese[1] — [1]IMCN-NAPS, Université catholique de Louvain, Place Croix du Sud 1, B-1348 Louvain-la-Neuve, Belgium — [2]Département de physique, Université de Montréal, C.P. 6128, Succursale Centre-Ville, Montréal, Canada H3C 3J7

We use analytic multi-pole models in lieu of standard plasmon-pole models [PRB(RC), accepted (2011)] in order to capture the detailed frequency dependence of the screened Coulomb interaction in crystalline systems [pssb 248, 275 (2011)]. These are applied in a quasi-particle self-consistent GW scheme for the evaluation of the many-body quasi-particle bulk band structure of the transparent conducting oxide hosts ZnO, MgO, SnO and SnO2. Optical spectra obtained using the Bethe-Salpeter equation are compared with experiment and with methods utilising the orbitals and eigenenergies from computationally less demanding ground-state methods. Several current popular local and non-local ground-state DFT and generalised Kohn-Sham approaches like the LDA, GGA, meta-GGA, and COHSEX are tested in this way. These studies show that it is possible to obtain a good description of optical spectra with a reasonable computational effort.

DF 11.6 Wed 11:20 EB 107

Electronic structure of lanthanum bromide and strontium iodide from many-body perturbation theory calculations — •Paul Erhart[1,2], Daniel Åberg[2], and Babak Sadigh[2] — [1]Applied Physics, Chalmers University of Technology, Gothenburg, Sweden — [2]Lawrence Livermore National Laboratory, Livermore, California, USA

Rare-earth based scintillators represent a challenging class of scintillator materials due to pronounced spin-orbit coupling and subtle interactions between d and f states that cannot be reproduced by standard electronic structure methods such as density functional theory. In this contribution we present a detailed investigation of the electronic band structure of $LaBr_3$ using the quasi-p article self-consistent GW (scGW) method. This parameter-free approach is shown to yield an excellent description of the electronic structure of $LaBr_3$. Specifically we reproduce the correct level ordering and spacing of the 4f and 5d states, which are inverted with respect to the free La atom, the band gap as well as the spin-orbit splitting of La-derived states. We furthermore present electronic structure calculations using G_0W_0 for the important scintillator material SrI_2. We explicitly take into account spin-orbit coupling at all levels of the theory. Our results demonstrate the applicability and reliability of the scGW approach for rare-earth halides. They furthermore provide an excellent starting point for investigating the electronic structure of rare-earth dopants such as Ce and Er.

DF 11.7 Wed 11:40 EB 107

Circular Dichroism in Biological Photonic Crystals — •Matthias Saba[1], Michael Thiel[2], Mark Turner[3], Klaus Mecke[1], and Gerd Schröder-Turk[1] — [1]Theoretische Physik, Universität Erlangen, 91058 Erlangen, Germany — [2]Angewandte Physik & Center for Functional Nanostructures, KIT, 76128 Karlsruhe, Germany — [3]Centre for Micro-Photonics & CUDOS, Swinburne University of Technology, VIC 3122, Australia

We introduce a chirality index that measures the circular dichroism of chiral photonic crystals by quantifying the degree of circular polarisation of the photonic band structure eigenmodes [1]. Nature provides a variety of examples for structural color in bird feathers, beetle shells and butterfly wings. It is widely accepted that the green color of the butterfly callophrys Rubi is caused by the nanostructure of its chitin wing-scales. This structure is modelled by a Gyroid constant mean curvature body and acts as a photonic crystal [2]. Our method, backed up by an alternative numerical transmission calculation based on a scattering matrix approach, reveals strong circular dichroism of the chiral Gyroid photonic crystal in the near UV. This response is a remarkable finding for a photonic crystal made of air and chitin with a low dielectric contrast and suggests technological designs [3] as well as possible relevance for butterfly communication.

[1] M. Saba et al., Phys. Rev. Lett. 106, 103902 (2011)
[2] G.E. Schröder-Turk et al., J. Struct. Biol. 174(2), 290 (2011)
[3] M. D. Turner et al., Opt. Express 19, 10001 (2011).

DF 11.8 Wed 12:00 EB 107

Aufbau eines NOPA bei 208 kHz Wiederholrate für Röntgen-Pump-Probe Experimente am Synchrotron — •Mathias Sander, Hengameh Navirian, Peter Gaal und Matias Bargheer — Universität Potsdam, Karl-Liebknecht-Str- 24-25 14476 Potsdam

Wir verwenden einen nicht-kollinearen phasenangepassten optisch parametrischen Verstärker (NOPA) [1], der von einem faserbasierten Lasersystem mit einer einstellbaren Repitionsrate zwischen 200 kHz bis 25 MHz gepumpt wird, für hochsensitive Anrege-Abtast-Experimente. Das Lasersystem ist als Anregequelle für zeitaufgelöste Röntgendiffraktionsexperimente am Synchrotron BESSY II konzipiert. Die Emissionswellenlänge des Lasers von 1035 nm wird direkt zur Erzeugung eines Weißlicht-Kontinums in einem Saphir-Kristall verwendet. Im weiteren mehrstufigen Aufbau können so durchstimmbare Laserpulse im Bereich von 620 nm bis 970 nm erzeugt werden. Durch anschließende Wellenlängenkonversion dieser Pulse mittels zweiter und dritter Harmonischen sowie Summenfrequenzmischung lassen sich sogar Wellenlängen deutlich unter 300 nm erreichen. In diesem NOPA-Aufbau lassen sich Pulsdauern unter 20 fs bei Pulsenergien von ca. 850 nJ erreichen. Die Sensitivität des Aufbaus soll durch hochrepetitives scannen gesteigert werden. Zukünftig soll der Aufbau in Verbindung mit der Synchrotronquelle zur Untersuchung von nanostrukturierten Schichtsystemen und komplexen Materialien, z.B. Perovskit-Oxiden, verwendet werden.

[1] E. Riedle et al.,Optics Letters Vol. 33, No.2 (2008)

DF 12: Nano- and microstructured dielectrics

Time: Wednesday 12:25–12:45 Location: EB 107

DF 12.1 Wed 12:25 EB 107

Fiber based optical microcavities for spectroscopy of nanoscale systems — •David Hunger[1,2], Hanno Kaupp[1,2], Matthias Mader[1,2], Christian Deutsch[1,3], Jakob Reichel[3], and Theodor W. Hänsch[1,2] — [1]Ludwig-Maximilians-Universität München, Deutschland — [2]Max-Planck Institut für Quantenoptik, Garching, Deutschland — [3]Laboratoire Kastler Brossel, E.N.S, Paris, Frankreich

We introduce fiber-based Fabry-Perot optical microcavities [1] as a versatile tool to study the optical properties of individual nanoscale solid state systems. This type of cavity benefits from full tunability, free space access to cavity modes, a mode volume on the order of a few tens of wavelengths cubed, and optical quality factors exceeding 10^6. In our experiments we want to use these exceptional properties to study nanoscale systems with high sensitivity and to realize strong light-matter interactions.

We show first experimental results on absorption spectroscopy of individual gold nanoparticles and report first steps towards the observation of cavity enhanced emission of NV color centers in diamond.

[1] Hunger,Reichel *et al.*, NJP **12**, 065038 (2010)

DF 13: Poster II

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

DF 13.1 Wed 15:00 Poster E

Impedance spectroscopy of printable electrolytes: calculation of frequency dependent effective capacitance — •Anna Stoesser, Robert Kruk, Nina Schweikert, Subho Dasgupta, and Horst Hahn — Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

In this work firstly presented an ink-jet printed and electrochemically-gated inorganic oxide based FET where indium tin oxide(ITO) nanoparticles compose the active channel of the device. Due to extremely effective gating possible by the polymer electrolytes which closely follows the roughness of the nanoparticulate channel, we obtain a large value of field-effect mobility. However, a generally expressed concern is that the electrolyte-gated device speed is limited by the ionic mobility of the electrolyte. Therefore, we have investigated the conductivity and frequency dependent polarizability of the printable grade of solid polymer electrolyte using electrical impedance spectroscopy. The frequency-dependent effective capacitance of ITO electrodes is calculated. It is shown that if cut-off frequency is defined as $1/2\pi$RC then the value of cut-off frequency for our electrolyte can be as high as 40 kHz when the thickness of the printed electrolyte is about 100 nm. Electrolyte conductivity can be foreseen with regular optimization, therefore, it may be concluded that finally electrolytes would not limit the attainable max. speed for the device-type presented here. Thus, an improvement of resolution and positional accuracy in the printing process is believed to be the key in this case to increase the speed of such transistors from kHz to MHz regime.

DF 13.2 Wed 15:00 Poster E

Complex Impedance Model for Metal/Amorphous Semiconductor/Semiconductor (MASS) heterostructures — •Julian Alexander Amani, Tristan Koppe, Marc Brötzmann, Hans Hofsäss, and Ulrich Vetter — Georg-August-Universität Göttingen, II. Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

A complex impedance model for MASS heterostructures is developed and compared with voltage dependent impedance spectroscopy measurements of the metal/ta-C/Si system.

The dominant dc conduction process of ta-C is hopping of carriers and the ac conductivity follows the "universal power law" $\sigma \propto \omega^s$ with $s \approx 0.8$. Hence, ta-C is an exemplary disordered material enabling us to investigate the dielectric properties of this material class.

An equivalent circuit considering the dielectric properties and voltage dependence of an disordered material is presented and compared with complex impedance measurements of ta-C.

Metal/ta-C/Si systems with weakly doped silicon substrates show a rectifying behaviour. Adding a depletion layer equivalent circuit to the model gives a good agreement with the data obtained for measurements of those samples.

DF 13.3 Wed 15:00 Poster E

Frequency dependency of the complex elastic stiffnesses of some ferroelectric ceramics — •Ulrich Straube and Horst Beige — Institute of Physics, University Halle, Germany

Ferroelectric ceramic materials exhibit pronounced temperature dependencies of their dielectric properties. The dielectric spectroscopy is used in a broad frequency region with standard equipment to analyze the dielectric material properties. The elastic spectroscopy allows the determination of the elastic stiffness frequency dispersion, but rather different measurement techniques have to be applied for this purpose.

Examples of stiffness determinations with pulse ultrasound at 5 MHz and dynamical mechanical analysis in a frequency range of 0.01 Hz up to 10 Hz and temperatures from 170 K up to 420 K are presented. The investigation are performed using lead zirconium titanate and barium titanate stannate ceramics.

DF 13.4 Wed 15:00 Poster E

Electrical and Structural properties of thermally transformed high-k dielectric $Ba_{0.7}Sr_{0.3}O$ thin films on p-Si(100) — •Shariful Islam[1], Dirk Müller-Sajak[1], Alexandr Cosceev[2], Herbert Pfnür[1], and Karl R. Hofmann[2] — [1]Leibniz-Universität Hannover, Inst. f. Festkörperphysik — [2]Leibniz-Universität Hannover, Bauelemente der Mikro- und Nanoelektronik

Crystalline thin films of $Ba_{0.7}Sr_{0.3}O$ were tested as a high-k dielectric material deposited on p-Si(100) substrate. The valence band offset and conduction band offset between p-Si(100) and $Ba_{0.7}Sr_{0.3}O$ was $\sim$2.3eV and $\sim$1.0eV respectively.

It was observed that $Ba_{0.7}Sr_{0.3}O$ was stable up to 400^0C. At higher temperature silicon from the substrate diffuses into the oxide and forms a silicate, as found by XPS. SPA-LEED measurements showed that the silicate phase is amorphous once the reaction is completed (550^0C). Electron Energy Loss Spectroscopy (EELS) of this silicate phase revealed a higher band gap ($\sim$6eV) compared to crystalline $Ba_{0.7}Sr_{0.3}O$ ($\sim$4.3eV). XPS measurements prove that the silicate phase is more stable in ambient conditions than $Ba_{0.7}Sr_{0.3}O$. Extrapolations of dielectric constants at various conditions predict that also this silicate may be usable as a high-k dielectric.

DF 13.5 Wed 15:00 Poster E

Oxygen Related Defects and the Reliability of High-κ Dielectric Films in Field Effect Transistors: An Investigation beyond Density Functional Theory — •Ebrahim Nadimi[1,2], Rolf Öttking[2], Philipp Plänitz[2], Martin Trentzsch[3], Torben Kelwing[3], Rick Carter[3], Christian Radehaus[2], and Michael Schreiber[1] — [1]Institut für Physik, Technische Universität Chemnitz, D-09107, Chemnitz Deutschland — [2]GWT-TUD GmbH Geschäftsstelle Chemnitz, Annaberger Str. 240, 09125 Chemnitz, Deutschland — [3]Global Foundries, D-01109, Dresden Deutschland

The introduction of high-κ (HK) gate dielectrics and metal gate in silicon field effect transistors has created many challenges amongst others the reliability of the gate dielectric. Bias temperature instability (BTI) and stress induced leakage current (SILC) are the key degradation characteristics. The community agrees about the important role of oxygen related defects in the degradation process of HK dielectrics. In this work, ab initio methods are applied to investigate oxygen vacancies as the most important defects in Hf-based dielectrics. Atomic structure, formation energy and electronic structure of these defects are investigated at the level beyond density functional theory using the exact-exchange hybrid functional. We also propose a defect generation mechanism, which could explain the relatively low defect activation energies obtained experimentally. The passivation of the oxygen vacancies by means of different dopants is also investigated and the results are compared. This work was supported by the Sächsische AufbauBank under HEIKO project Grant No. 1000648806/626.

DF 13.6 Wed 15:00 Poster E

Restoring the k value in carbon depleted ultra low k surfaces by the silylation of hydroxyl groups with N-trimethylsilylimidazole and dimethyldiacetoxysilane. — Oliver Böhm[1,2], Roman Leitsmann[2], Philipp Plänitz[2], •Christian Radehaus[2], Matthias Schaller[3], and Michael Schreiber[1] — [1]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz — [2]GWT-TUD GmbH, Material Calculation, Annaberger Str. 240, 09125 Chemnitz, Germany — [3]GLOBALFOUNDRIES Dresden Module Two GmbH & Co. KG, Germany

To reduce the resistance capacitance delay of integrated circuits, ma-

terials with a small k-value - so called ultra low k materials (ULK) - are used as interlayer dielectrics. An important fabrication step in the semiconductor industry is the etching of the trenches, which leads to a carbon depletion and a formation of hydroxyl groups in the ULK material. This results in a moisture uptake and hence an increased k value. To restore the k value, a silylation of the hydroxyl groups can be done. We investigate the silylation of hydroxyl groups by the chemicals N-trimethylsilylimidazole (TMSIM) and dimethyldiacetoxysilane (DMDAS). In particular we use density functional theory to study the different reaction mechanisms. To determine the minimum energy reaction paths as well as transition states, we use the nudged elastic band method. We found significant differences in the activation barriers, reaction energies and the formation of pre and post reaction complexes of TMSIM and DMDAS.

DF 13.7 Wed 15:00 Poster E

Verzögerte Kristallisation ultradünner Gd2O3 Schichten auf Si(111) beobachtet mittels in-situ Röntgenbeugung — •Michael Hanke, Vladimir Kaganer, Oliver Bierwagen, Michael Niehle und Achim Trampert — Paul-Drude-Institut Für Festkörperelektronik, Hausvogteiplatz 5-7, D-10117 Berlin

We studied the early stages of Gd2O3 epitaxy on Si(111) in real time by synchrotron-based in-situ high resolution x-ray diffraction and by reflection high-energy electron diffraction. A comparison between model calculations and the measured x-ray scattering, and the change of reflection high-energy electron diffraction patterns both indicate that the growth begins without forming a threedimensional crystalline film since the very first monolayers are not in perfect registry among each other. A cubic bixbyite structure of Gd2O3 appears only after a few monolayers of deposition.

DF 13.8 Wed 15:00 Poster E

Effect of high-frequency on etching of SiCOH films in CHF3 dual-frequency capacitively coupled plasmas — •Yijun Xu — II. Physikalisches Institut, Universität Göttingen, Friedrich- Hund-Platz 1, 37077 Göttingen, Germany — School of Physics Science and Technology, Jiangsu Key Laboratory of Thin Films, Soochow University, Suzhou 215006, People's Republic of China

The effect of high-frequency (HF) frequency on etching characteristics of SiCOH films in a CHF3 dualfrequency capacitively couple plasma driven by 13.56 MHz/2 MHz, 27.12 MHz/2 MHz or 60 MHz/2 MHz sources was investigated in this work. The surface structure of the films after etching and the CHF3 discharge plasma were characterized. The increase of HF frequency reduced the critical HF power for the etching, suppressed the C:F deposition at the surface of etched films, and improved the etching of SiCOH films. The improvement of etching was attributed to the increase of ions energy and F concentration at high HF frequency.

DF 13.9 Wed 15:00 Poster E

Ionic-Liquid Promoted Crystalline β Phase in Polyvinylidene Fluoride Nanofilms — •Alexander Lack, Feipeng Wang, Peter Frübing, Werner Wirges, and Reimund Gerhard — Applied Condensed-Matter Physics, Department of Physics and Astronomy, Faculty of Science, University of Potsdam, Karl-Liebknecht-Strasse 24-25, 14476 Potsdam-Golm, Germany

Up to now it is immensely difficult to obtain sub-micrometer thin films of polyvinylidene fluoride (PVDF) in the ferroelectric β phase. We present a novel way to achieve β-phase PVDF sub-micrometer thin films that were obtained by spin coating from a solution containing a small portion of the ionic liquid 1-ethyl-3-methylimidazolium nitrate [EMIM][NO_3]. After drying and annealing at temperatures above 100 °C the films showed strong ferroelectric hysteresis with a remanent polarization of maximum 76 mC/m^2 and a coercive field of 200 MV/m. The pyroelectric coefficient was measured to 17 μC/(m^{2}K) at 30 °C. The impact of [EMIM][NO_3] on the crystallization behavior of PVDF, with particular attention to the occurrence and ratio of the ferroelectric β phase, was confirmed using infrared spectroscopy and X-ray diffraction. The surface morphology was determined using atomic force microscopy and scanning electron microscopy. They show that under the influence of ionic liquids no α-phase spherulitic crystallites are visible and the size of the crystalline regions decreases from about 10 to 2 μm. The ferroelectric β phase is assumed to be promoted by Coulomb interaction between NO_3^- anions and the molecular dipoles of PVDF.

DF 13.10 Wed 15:00 Poster E

Correlation between structural and ferroelectric properties of $BaTiO_3$ thin films — •Anja Herpers[1], Regina Dittmann[1], Daesung Park[2], Joachim Mayer[2], and Rainer Waser[1] — [1]Peter Grünberg Institut 7, Electronic Materials, Forschungszentrum Jülich GmbH, 52428 Jülich — [2]Gemeinschaftslabor für Elektronenmikroskopie, RWTH Aachen University, Ahornstraße 55, 52074 Aachen

Point as well as extended defects in ferroelectric thin films are expected to have a strong influence on their ferroelectric properties. We investigated in detail the influence of growth conditions on the crystal structure of $BaTiO_3$ (BTO) thin films and its influence on the ferroelectric hysteresis loops and the leakage currents.

We performed detailed experiments to distinguish between the different types of defects by varying the pulsed laser deposition (PLD) parameters and the post annealing conditions. Furthermore, systematic studies of the influence of the growth kinetics on the oxygenation state of the thin films were performed and related to defect chemistry models. These investigations were complemented by high resolution transmission electron microscopy analysis of the atomic structure of the thin films and different types of electrode interfaces.

We succeeded to obtain closed hysteresis loops with a remanent polarization of 30μC/cm^2 for a 30nm thick BTO thin films stacked between $SrRuO_3$ and Pt electrodes.

DF 13.11 Wed 15:00 Poster E

Identification of electronic defect states in perovskite oxides — •Elke Beyreuther, Jana Becherer, Stefan Grafström, and Lukas M. Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden, Germany

Perovskite oxide heterojunctions such as the $LaAlO_3/SrTiO_3$ interface have attracted enormous scientific interest due to their unexpected and tunable physical properties but equally because of their technological promises with respect to all-oxide integrated nanodevices. Among other unresolved issues, the detailed physical understanding of the electronic defect structure at these interfaces is indispensable.

We adopt here the surface photovoltage (SPV) method to inspect the surfaces and interfaces of $SrTiO_3$ (STO), which serves as our model perovskite. SPV has already substantially contributed to the analysis of III-V and II-VI semiconductor interfaces, both through spectrally and temporally resolved investigations. Here, we investigated the STO system by acquiring static and transient SPV data over a wide wavelength range and for various light intensities. This allowed us to identify and quantify defect states across the STO band gap, and to derive parameters of distinct states such as optical cross sections and time constants. The feasibility and general possibilities of applying SPV for the analysis of perovskite heterostructures will be discussed.

DF 13.12 Wed 15:00 Poster E

Raman spectroscopic investigations of $CoFe_2O_4$ and $NiFe_2O_4$ epitaxial sub-micron structures — •Cameliu Himcinschi[1], Ionela Vrejoiu[2], and Andreas Talkenberger[1] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09596 Freiberg — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle

$CoFe_2O_4$(CFO) and $NiFe_2O_4$(NFO) are insulating ferrimagnetic spinel oxides that are attractive for application in magneto-electric oxide heterostrucuture devices. CFO and NFO epitaxial thin films were grown on Nb-doped $SrTiO_3$(100) substrates by pulsed-laser deposition. For the fabrication of ordered arrays of sub-micron structured CFO and NFO a SiN stencil mask was used. In this work we present an investigation of the CFO and NFO thin films and structures by Raman spectroscopy. The Raman spectra of CFO and NFO thin films indicate the formation of a spinel structure with symmetry lower than the cubic inverse spinel one. The assignment of the Raman modes was done by employing different polarization scattering configurations. Similar spectra were measured also for the structured arrays suggesting the preservation of the structure observed in the epitaxial thin films. The degree of disorder in the cation distribution in the octahedral sites is discussed based on the broadening of the Raman peaks.
This work is supported by the German Research Foundation DFG HI 1534/1-1.

DF 13.13 Wed 15:00 Poster E

Production of sub-μm to cm structures on fused silica by laser-induced front side etching using self-regenerating adsorber layer (SAL-LIFE) — •Pierre Lorenz, Martin Ehrhardt, and Klaus Zimmer — Leibniz-Institut of Surface Modification, Per-

moserstr. 15, 04318 Leipzig, Germany

Laser-induced front side etching (LIFE) is a method for production of 3D structures in dielectric materials over a wide lateral and vertical size range. Within this study the continuous laser-induced front side etching of fused silica with self-regenerating adsorber layers (SAL-LIFE) is presented using nanosecond KrF excimer laser radiation (λ = 248 nm, Δt_p = 25 ns). The sample was positioned in a vacuum chamber which was loaded by toluene gas and the gas phase induced the self-regenerating adsorber layer on the sample surface. For the etching process, the laser beam was focused onto the sample surface through the gas. The SAL-LIFE method allows the production of well-defined nm-precision etched surface structures over a large etching depth range from nm to a few hundred μm as well as a large lateral etching region from sub-μm to a few cm. A surface roughness down to 1 nm can be achieved. The treated fused silica was analysed with microscopic (white light interferometry, scanning electron microscopy (SEM)) and spectroscopic methods (X-ray photoelectron spectroscopy (XPS)).

DF 13.14 Wed 15:00 Poster E

Correlation between size evolution and optical properties of ion beam synthesized silver nanoclusters in lithium niobate — •Jura Rensberg, Steffen Milz, Carsten Ronning, and Werner Wesch — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Metal nanoclusters embedded in various dielectrics gained a lot of interest for plasmonic applications like optical filters or plasmonic waveguides in the last two decades. Because of its unique electro-optical and nonlinear optical properties, lithium niobate ($LiNbO_3$) is one of the most important materials for integrated optics. Noble metals like silver are of particular relevance for cluster formation in $LiNbO_3$, because of its distinctive surface plasmon resonance (SPR) located in the visible spectral range. We have implanted 380 keV Ag^+ ions up to an ion fluence of 1x10^{17} cm^{-2} into $LiNbO_3$ at room temperature and 673 K. Isochronal rapid thermal annealing as well as isothermal annealing were performed in the temperature range of 573 K to 1173 K, resulting in the formation of silver nanoclusters with different size distributions and a reduction of irradiation damage. The samples were analyzed by means of RBS-channeling, and STEM as well as optical spectroscopy. The correlation between structural and optical properties will be discussed in detail in this study.

DF 13.15 Wed 15:00 Poster E

Coupling nanoscale solid state systems to optical fiber microcavities — •Hanno Kaupp[1,2], David Hunger[1,2], Matthias Mader[1,2], Christian Deutsch[1,3], Jakob Reichel[3], and Theodor W. Hänsch[1,2] — [1]Ludwig-Maximilians-Universität München, Deutschland — [2]Max-Planck-Institut für Quantenoptik, Garching, Deutschland — [3]Laboratoire Kastler Brossel, E.N.S., Paris, Frankreich

Optical fibers with machined and coated endfacets can serve as high reflectivity mirrors to build low loss microcavities [1]. Featuring a small mode volume on the order of a few tens of cubic wavelengths, optical quality factors exceeding 10^6, and free space accessability to the cavity modes, they are well suited to study nanoscale systems with high sensitivity. We will present first steps towards coupling a nitrogen-vacancy centers in nanodiamonds to the fiber cavity. First experimental results on absorption spectroscopy with gold nanoparticles will be discussed.

[1] Hunger, Reichel et al., NJP 12, 065038 (2010)

DF 13.16 Wed 15:00 Poster E

First principles study of the magneto-optical Kerr effect in $TbAl_3(BO_3)_4$ — •Udo Schwingenschlögl, Yasir Saeed, and Nirpendra Singh — KAUST, PSE Division, 23955-6900 Thuwal, Kingdom of Saudi Arabia

The electronic and optical properties of $TbAl_3(BO_3)_4$ are determined using density functional theory. The calculated total magnetic moment of 5.96 μ_B is close to the expected moment of Tb^{3+}. The frequency dependent dielectric function, refractive index, extinction coefficient, absorption, optical reflectivity, and energy loss function are explained in terms of the transitions between the valence and conduction bands. We find very high Kerr angles for ultraviolet light and potential for extension, even into the visible range by band structure design.

Reference: J. Appl. Phys., in press, doi:10.1063/1.3662176

DF 13.17 Wed 15:00 Poster E

Heat relaxation and transport in dielectrics: the density dependent two temperature model — •Anika Scholtes[1], Orkhan Osmani[1,2], and Bärbel Rethfeld[1] — [1]TU Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Universität Duisburg-Essen, 47048 Duisburg, Germany

During the irradiation of dielectrics and semiconductors with a laser pulse or a swift heavy ion, electrons are excited from the valence band into the conduction band, thus creating electron-hole-pairs. The excited electronic system interacts with the phononic system by electron-phonon-coupling. For laser-irradiated metals, the two temperature model (TTM) introduced in [1] describes the temporal and spatial evolution of electronic and phononic temperature. Considering dielectrics and semiconductors with an initially negligible free electron density, it is also important to account for the transient electronic density in the conduction band. A first approach to obtain the evolution of the phononic as well as the electronic temperature, which also accounts for the change in the density, was given in [2]. Here, we modified this approach to fully account for the energy conservation and present the influence of the impact ionization and Auger recombination on the electronic density and temperature dynamics for the case of laser-irridiation of Silicon.

[1] S.I. Anisimov, B.L. Kapeliovich, and T.L. Perel'man. *Sov. Phys. JETP* **39**, 375 (1974).

[2] H.M. van Driel. *Phys. Rev. B* **35**, 8166 (1987).

DF 13.18 Wed 15:00 Poster E

Transient absorption in $Sn_2P_2S_6$ induced by sub-100-fs light pulses — •Volker Dieckmann[1], Holger Badorreck[1], Mirco Imlau[1], and Alexandr Shumelyuk[2] — [1]Department of Physics, University of Osnabrück, Germany — [2]Institute of Physics, National Academy of Science, Kyiv, Ukraine

The interaction of sub-100-fs light pulses with single crystals of nominally undoped $Sn_2P_2S_6$ is studied in the NIR spectral range (590 − 1630 nm) [1]. A predominant contribution of the two-photon absorption (TPA) is verified. The TPA coefficient β increases in a superlinear way for photon energies $\hbar\omega$ exceeding $E_g/2$; for any photon energy it is nearly independent of propagation direction and polarization of the incident beam. The TPA coefficient saturates at a maximum value of $\beta \approx 8\,\mathrm{cm\,GW^{-1}}$ at $\hbar\omega \approx 1.8\,\mathrm{eV}$. It drops when reaching the bandgap E_g. The TPA coefficients are higher by a factor of two than the values reported for other wide bandgap ferroelectrics, such as $LiNbO_3$, while being lower in comparison to semiconductor crystals. Using pump-probe measurements at 626 nm, a transient absorption is observed that persists for probe pulse delays much longer than the pump pulse duration, up to 2.5 ns. Such transients are typical for a variety of wide bandgap ferroelectrics, where they are described by optically generated polaronic states. We discuss our results in the framework of the microscopic structure of $Sn_2P_2S_6$ with emphasis on the optical generation of S^- small hole polarons. Financial support by the DFG (IM 37/9-1, INST 190/137-1) is gratefully acknowledged.

[1] M. Imlau et al. Opt. Mater. Express 1, 953 (2011)

DF 13.19 Wed 15:00 Poster E

Transient absorption and nonlinear refractive index changes in nominally pure, thermally reduced $LiNbO_3$ induced by sub-100-fs light pulses — •Holger Badorreck, Volker Dieckmann, Pia Baeune, and Mirco Imlau — Department of Physics, University of Osnabrück, Germany

Nominally undoped lithium niobate—as grown and thermally reduced—is of great interest for ultrafast optical devices due to its polaronic features. With formation times in the sub-ps-range short-lived small polarons can be generated in reduced samples by optical gating of bipolarons due to single photon absorption. Simultaneously, formation of small hole polarons by two-photon-absorption is observed. In this work nonlinear absorption and refractive index changes due to exposure to sub-100-fs light pulses of 488 nm are presented in presence of a considerable number density of bipolarons. It is found that the two-photon absorption coefficient is not affected by the thermal reduction procedure, whereas the nonlinear refractive index change is considerably smaller in the reduced sample compared to the unreduced one. We further present our results on the study of the transient absorption in the blue and NIR spectral range by means of fs-pump-probe technique. The influence of the thermal reduction procedure on lifetime and densities of electron and hole polarons is discussed.

Financial support by the DFG (IM 37/5, INST 190/137-1) is gratefully acknowledged.

DF 13.20 Wed 15:00 Poster E

Light-induced absorption spectroscopy in niobate, titanate and borate crystals — •Andreas Buescher[1], Hauke Bruening[1], Bettina Schoke[1], Christoph Merschjann[2], Stefan Torbruegge[1], Gabor Corradi[3], Susanne Hoffmann-Eifert[4], and Mirco Imlau[1] — [1]Department of Physics, University of Osnabrück, Germany — [2]Helmholtz-Zentrum für Materialien und Energie, Berlin, Germany — [3]Research Institute for Solid State Physics and Optics, Budapest, Hungary — [4]Institut für elektronische Materialien, Forschungszentrum Jülich, Germany

Light-induced absorption spectroscopy (LIAS) is a powerful tool for investigation of wide bandgap oxide materials. In this contribution, we will review the results in the niobates $LiNbO_3$ and $KNbO_3$ as well as in $SrTiO_3$ and β-BaB_2O_4. In $LiNbO_3$, we study the complex interplay of two-photon excitation of small hole and bound polarons and the optical gating of bipolarons into free and bound polarons. In $KNbO_3$, we deal with one electron and one hole polaron allowing for the development of a new model for thermally activated polaron hopping giving access to new microscopic parameters. $SrTiO_3$, widely discussed as a memristor material, is studied using LIAS to get insight into the charge transport properties of this material taking into account the model of extended defects. In β-BaB_2O_4 polarons are discussed as the origin of laser damage. We face the problem as a result of the high photon-flux showing the limitations of this measurement technique.

Financial support by the DFG (IM37/5 and INST190/137-1) and DAAD (50445542) is gratefully acknowledged.

DF 13.21 Wed 15:00 Poster E

Light-induced linkage isomerization by ultrafast mid-infrared spectroscopy in sodium nitroprusside on the 100 fs time domain — •Felix Freytag, Kristin Springfeld, Volker Dieckmann, and Mirco Imlau — Department of Physics, University of Osnabrück, Germany

Today's information storage and telecommunication industry strongly demands for novel devices to increase storage densities and transmission speed in optical networks. A promising approach is the control of light by light using molecular compounds offering ultrafast photochromism and -refraction on the sub-ps time scale. Nitroprusside compounds have been shown to allow for these features based on a light-induced linkage isomerization [1]. Recently, its time constant has been reported to be less than 200 fs by means of VIS-pump-probe technique [2]. However, such structural alterations have not been proven in the compound by direct measurements on the sub-ps time scale. For studying selected vibrational modes at $\nu \approx 1950\,\mathrm{cm}^{-1}$ of sodium nitroprusside, we use frequency-resolved infrared spectroscopy. The transmission of mid-infrared $\tau \approx 150$ fs pulses is detected by a multichannel MCT detector as a function of time delay to an intense VIS pump pulse of $\tau \approx 100$ fs duration. We will present first results on our studies of the light-induced changes of such vibrational modes on the 100 fs time scale. Financial support by the DFG (IM 37/5, INST 190/137-1) and the DAAD (50445542) is gratefully acknowledged.

[1] Imlau et al., Appl. Phys. B, 68, 877 (1999)
[2] Schaniel et al., Phys. Chem. Chem. Phys., 12, 9029 (2010)

DF 13.22 Wed 15:00 Poster E

Hydrophones based on photonic crystals — Timm Schaer[1,2], •Juliane Tschentscher[2], and Mirco Imlau[2] — [1]ATLAS ELEKTRONIK GmbH, Sebaldsbrücker Heerstr. 235, D-28309 Bremen — [2]Department of Physics, University of Osnabrück

Hydroacoustic sensors commonly consist of piezoelectric ceramics that convert acoustical pressure to electric signals. However, their application in the deep sea (>1800 m depth) with remotely-operated undersea vehicles (ROV) is limited because of large signal losses in copper based connecting wires. In this context, fiber-based photonic networks that include optical hydrophones represent a promising solution. Here, we focus on the application of photonic crystals as highly sensitive sensor elements in hydroacoustic devices. Photonic crystals are artificial structured materials on the scale of light wavelength. Because of their unique sensitivity to alterations in the periodic structure, they are particularly suited for the detection of mechanical pressure and, hence, for the detection of acoustic waves. We have selected polymethymethacrylat (PMMA) as base material because of its Young's modulus, transparency and chemical stability. We present our results on the recording of quasi-periodic structures by means of exposure to ns- and fs-laser pulses. The structures that allow the control of light at the telecommunication wavelength (1.55 μm) are analyzed by photo spectroscopy and light diffraction. The response of the device to dynamic changes of mechanical pressure under seawater conditions is discussed.

Financial support by the DFG (IM37/5, INST 190/137-1) is gratefully acknowledged.

DF 13.23 Wed 15:00 Poster E

Size-dependent optical properties of polar oxide $BaTiO_3$ nanocrystals applied for cell imaging — •Pia Bäune[1], Mirco Imlau[1], Karsten Kömpe[2], and Jacob Piehler[2] — [1]Fachbereich Physik, Universität Osnabrück — [2]Fachbereich Biologie/Chemie, Universität Osnabrück, Germany

Polar oxide nanocrystals have been introduced as novel class of optical markers for cell imaging in biophotonics. Based on frequency conversion they obey interesting, outstanding properties in comparison with imaging techniques via fluorescence and resonance spectroscopy. For instance, pump- and probe-photon energies are spectrally separated, the crystals show no photobleaching and/or photoblinking, and coherent light is generated with anisotropic radiation characteristics. Thus, polar oxide nanocrystals are promising candidates for continuous three-dimensional detection of both position and orientation of markers in biological cells. In this contribution we present our studies on the size-dependent optical properties of $BaTiO_3$ nanocrystals by means of frequency conversion techniques. $BaTiO_3$ nanocrystals have been synthezised with colloidchemical methods taking hydrothermal and solvothermal methods for bulk crystal growth into account. We focus on photodegradation phenomena that relate to the nanocrystal surfaces as a function of nanoparticle size. Our results are compared with $BaTiO_3$ bulk crystals with respect to SHG efficiency and the processes of laser-induced surface damages. Surface modification by SiO_2 or polymers (PEG, PVB) is proposed and discussed taken the physiological environment in cells into account.

DF 13.24 Wed 15:00 Poster E

Adaptive Amplitude Filters for Smaller Feature Sizes in Direct Laser Writing — Erik Waller and •Georg von Freymann — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern

Direct-Laser-Writing is an established technique for the fabrication of almost arbitrary three-dimensional structures in photo resists. These are locally polymerized via two-photon polymerization. The fundamental building block - the so called voxel (volume pixel) - is a volume defined by the iso-intensity surfaces in the focal spot. This voxel is an ellipsoid, defined by the numerical aperture of the microscope objective and the refractive index of the photo resist. The resulting axial elongation is disadvantageous for isotropic features. To overcome this problem, so called shaded-ring filters have been reported. Recently, stimulated-emission-depletion inspired lithography has been demonstrated to yield aspect ratios of one. Corresponding setups require phase masks and an additional laser source. Here, we show that spatial light modulators can be employed to implement shaded-ring filters to decrease the aspect ratio. However, so far shaded-ring filter have to not been able to generate aspect ratios close to one with acceptable side lobe levels. We therefore suggest an adaptive amplitude filter allowing for voxels with an aspect ratio of one, regardless of the scanning direction. This adaptive filter consists of a variable slit with unity transmission imaged onto the entrance pupil of a high numerical aperture objective. We show numerical calculations and experimental data demonstrating the effectiveness of this approach.

DF 13.25 Wed 15:00 Poster E

Strukturierte Materialmodifikationen in optischen Kristallen mittels eines Hochenergie Helium-Microbeams — •Niels L. Räth, Johannes Goetze, Konrad Peithmann und Karl Maier — Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn

Optische Kristalle wie Lithiumniobat oder Lithiumtantalat sind äußerst interessant für eine Vielzahl optischer Anwendungen.

Hochenergetische, leichte Ionen, die derartige Kristalle durchstrahlen, verursachen langzeitstabile Modifikationen des Brechungsindexes und reduzieren die Koerzitivfeldstärke E_C.

Um die Materialen im Mikrometerbereich derart strukturieren zu können, wird der Ansatz eines Hochenergie Helium-Microbeams verfolgt. Am Isochron-Zyklotron des Helmholtz-Instituts für Strahlen- und Kernphysik wird dazu mittels ionenoptischer Abbildung ein maskierter Ionenstrahl stark verkleinert auf die Probe abgebildet.

Es werden Berechnungen, Aufbau und erste Resultate vorgestellt.

DF 13.26 Wed 15:00 Poster E

Impulsive stimulated Raman scattering on phonon-polaritons in oxides — •Jewgeni Goldshteyn[1], Daniel Schick[2], Andreas Paulke[2], Peter Gaal[2], and Matias Bargheer[1,2] — [1]Helmholtz Zentrum Berlin, Albert Einstein Str. 15, 12489 Berlin, Germany — [2]Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany

This contribution presents a time-resolved study of phonon-polariton dynamics in various materials like tetragonal $LiNbO_3$ and quasi-cubic $SrTiO_3$. We excite discrete modes by Impulsive Stimulated Raman Scattering (ISRS) using a k-selective transient grating technique. The excitation is probed by means of a second Raman scattering event, by detection of the four-wave-mixing signal in a box-car geometry. One virtue of our setup is the frequency-resolved detection of the scattered probe pulse, which allows for a measurement of stokes- and anti-stokes shifts of the probe light. The excitation process is presented thoroughly. In particular the transient atomic displacement and the sample symmetry are discussed. Further, we discuss implications on future ultrafast x-ray diffraction experiments to probe Raman excited modes.

DF 13.27 Wed 15:00 Poster E

Linear and non-linear optical properties of Lithium niobate — •Arthur Riefer[1], Simone Sanna[1], André V. Gavrilenko[2], and Wolf Gero Schmidt[1] — [1]Theoretische Physik, Universität Paderborn, 33095 Paderborn, Germany — [2]Norfolk State University, Center for Materials Research, VA 23504 Norfolk, USA

Lithium niobate (LN) is one of the most important ferroelectric materials and the most important optic material. Given the vast range of LN applications, our knowledge about its electronic and optical properties is surprisingly limited. Besides many experiments focusing on the onset of the absorption, we are aware of only two studies that address the absorption in the vacuum ultraviolet (VUV) domain [1,2]. Furthermore, theoretical works investigating the electronic and optical properties beyond the single-particle picture are rare[3,4]. Concerning the non-linear optical properties, only a single theoretical work exists [5]. Thus, in this work we use a quasiparticle band structure based on parameter-free GW calculations for setting up the excitonic Hamiltonian, determine the (linear) optical spectra, and compare to the experimental available spectra [1]. We also present a second-harmonic generation (SHG) spectrum for LN.

[1] A. M. Mamedov *et al.*, Appl. Phys. A **34**, 189 (1984)
[2] E. Wiesendanger *et al.*, Sol. State Commun. **14**, 303 (1974)
[3] W. G. Schmidt *et al.*, Phys. Rev. B **77**, 035106 (2008)
[4] C. Thierfelder *et al.*, phys. stat. sol. (c) **7**, 362 (2010)
[5] H. Akkus *et al.*,Int. J. Nanoelectronics and Materials **3**, 53 (2010)

DF 13.28 Wed 15:00 Poster E

Lithium tantalate electronic and optical properties calculated from first principles — •Arthur Riefer, Simone Sanna, and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn, 33095 Paderborn, Germany

Ferroelectric materials like Lithium tantalate (LT) are very important for the fabrication of non-linear optical and electro-optical devices. Despite its huge range of applications first principles studies including many-body interactions in the electronic structure and optical spectra of ferroelectrics are rare[2,3]. In particular for LT we are not aware of calculations going beyond density functional theory (DFT). In order to contribute to a better understanding of the LT electronic and optical properties we calculate its quasiparticle band structure within the GW approximation for the electronic self-energy. The optical response is calculated from a Bethe-Salpeter-type approach, thus including excitonic and local-field effects from first principles. The results are compared to similar calculations for other ferroelectric materials like Lithium niobate (LN). Also we present spectra for composite materials consisting of both LN and LT.

[1] Y. Xu, *Ferroelectric materials and their applications*, North-Holland, 1991
[2] W. G. Schmidt *et al.*, Phys. Rev. B **77**, 035106 (2008)
[3] C. Thierfelder *et al.*, phys. stat. sol. (c) **7**, 362 (2010)

DF 14: Poster III – 100 years since the Laue experiment: Topical aspects of diffraction and scattering (Joint Session KR, BP, CPP, DF, GP, MA, MI, MM)

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

DF 14.1 Wed 15:00 Poster E

Clip - The Cologne Laue Indexation Program — •Olaf J. Schumann — Fraunhofer-Institut für Naturwissenschaftlich-Technische Trendanalysen, Euskirchen, Deutschland — II. Physikalisches Institut, Universität zu Köln, Germany

The Cologne Laue Indexation Program is a software for the analysis and simulation of Laue images.

Clip features a modern graphical user interface, could read a large variety of image formats and allows to mark spots *and* zones in a recorded image. These could be used for automatic indexation of the image for arbitrary crystal symmetries and refinement of lattice constants and projection plane parameters. Clip helps with the alignment of the crystal to a desired orientation. It is an open source software (GPL) written in C++ and the cross platform toolkit Qt and runs on Windows, Linux and Mac OS X.

DF 14.2 Wed 15:00 Poster E

A new access to extinction corrections — •Anne K. Hüsecken and Ullrich Pietsch — Naturwissenschaftlich Technische Fakultät, Fachbereich Physik, Universität Siegen, D-57068 Siegen, Germany

In x-ray crystal structure analysis a problem, called extinction, occurs due to multiple scattering in crystals. Over the years several extinction correction theorems have been formulated, but the used parameters have never been proved to be valid for a certain crystal under investigation. Perfect crystals scatter according to the dynamical theory (I~|F|) and imperfect crystals or ideal mosaic crystals due to the kinematical theory (I~|F|*). In most cases, the measured intensities of real crystals are in between both cases and an extinction correction is needed to fulfil the kinematic approach. Present theories dealing with extinction corrections are based on the approach of a mosaic crystal and describe x-ray scattering in terms of the kinematic approach using certain "correction terms" to implement the structure of a real crystal. The mosaic blocs within a real crystal are misorientated to each other and are affected by lattice strain. In addition both 3D shape and size of the blocs are not known. All these parameters can be determined by high-resolution x-ray diffraction techniques performing ω- and ω-2θ-scans through certain reciprocal lattice points. The measured parameters can be used to determine extinction. Our aim for crystallography is to perform these scans only for a few reflections, make a short analysis, to get the size, misorientation and lattice strain of the mosaic blocs. With these parameters it should then be possible to decide which one is the best extinction correction to use.

DF 14.3 Wed 15:00 Poster E

Evaluation of interfacial orientation information from 3D X-Ray diffraction contrast tomography in and its application in a mesoscale grain coasening model — •Melanie Syha, Fabian Sehn, Andreas Trenkle, and Daniel Weygand — Karlsruher Institut für Technologie, IAM

The orientation information from 3D X-Ray diffraction contrast tomography investigations in polycrystalline $SrTiO_3$ ceramics was evaluated before and after annealing. Special emphasis was put on local interface orientations, showing a preference for <100> orientated interfaces that increases during microstructural evolution. Moreover the data was used to investigate orientation dependent relative interface mobilities. The results are discussed in the context of the abnormal growth behavior found in $SrTiO_3$ and used to adapt a mesoscale grain coarsening model to more realistic simulations of microstructure evolution in this material.

DF 14.4 Wed 15:00 Poster E

Inter-layer disorder in sodium cobaltate — •David Jonathan Pryce Morris[1], Alan Tennant[1,2], Klaus Seiffert[1,3], Esther Dudzik[1], Dharmalingam Prabhakaran[4], Jon Goff[5], Michel Roger[6], and Jon Wright[7] — [1]Helmholtz-Zentrum Berlin, Germany — [2]TU-Berlin, Germany — [3]Kiel University, Germany — [4]Oxford University, UK — [5]Royal Holloway, University of London, UK — [6]CEA-Saclay, France — [7]ESRF, France

Sodium Cobaltate is a layered material which has been studied as a potential battery material, has shown good thermoelectric properties and becomes superconducting when hydrated. The physical properties are dependent on sodium content and the ordering of sodium ions. Sodium ordering in NaxCoO2 has previously been observed to have long-range order. Using x-ray diffraction we have observed a phase with long-range in-plane order and inter-layer disorder. Here we will present the data giving a possible structural interpretation.

DF 15: Dielectric and ferroelectric thin films

Time: Thursday 9:30–11:35 Location: EB 107

Invited Talk DF 15.1 Thu 9:30 EB 107

Dielectric perovskite oxides: Always good for a surprise — •Annette Bussmann-Holder — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Deutschland

Dielectric perovskite oxides exhibit multiple complex phases which vary from purely displacive to order/disorder driven to precursor dynamics. Four special cases are in the focus of this talk: the cases of $BaTiO_3$, relaxor ferroelectrics, $SrTiO_3$ and its isotope induced ferroelectric state, and finally $EuTiO_3$ and its mixed crystals with $SrTiO_3$. It is shown, that for all these compounds a single model can account for the very different dynamical behaviour and that coexistences and crossovers in the dynamics occur which invalidate categorizing dielectric perovskites.

5 min. break

DF 15.2 Thu 10:15 EB 107

Strain effects in ferroelectric thin films: the impact on the switching kinetics of Pb(Zr,Ti)O_3 — •Andreas Herklotz[1,3], Michael D. Biegalski[2], Hans M. Christen[2], Ludwig Schultz[1], and Kathrin Dörr[3] — [1]IFW Dresden, 01171 Dresden, Germany — [2]Oak Ridge National Laboratory, Center for Nanophase Materials Sciences, 37831 Oak Ridge, TN, USA — [3]Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany

We present first results on the effect of biaxial strain on the switching of ferroelectric thin films. The strain state of epitaxially grown tetragonal and rhombohedral Pb(Zr,Ti)O_3 films is controlled directly and reversibly by the use of piezoelectric $Pb(Mg_{1/3}Nb_{2/3})_{0.72}Ti_{0.28}O_3$ (001) (PMN-PT) substrates. The ferroelectric switching behavior is investigated by pulsed electric polarization measurements.

At small external electric fields the films show switching characteristics consistent with a creep-like domain wall motion behavior. In this pinning regime we find a huge decrease of the switching time under compressive strain, i.e an acceleration of the switching kinetics. For larger external electric fields the domain wall motion turns into a depinning regime. The strain effect is changing to a moderate positive value, that is, the switching kinetics is slowed down under the influence of compressive in-plane strain. These results are found in tetragonal and rhombohedral films, thus revealing a general behavior that is not governed by the lattice symmetry or the domain pattern.

DF 15.3 Thu 10:35 EB 107

Nonlinear Dielectric Properties and Polarization in Ferroelectric P(VDF-TrFE) Copolymer Thin Films — •Danny von Nordheim, Steffen Hahne, and Bernd Ploss — Department of SciTec, University of Applied Sciences (FH) Jena, Carl-Zeiss-Promenade 2, 07745 Jena, Germany

VDF-TrFE copolymer ferroelectric thin films of molar composition 70/30 have been prepared by spin coating on glass substrate covered with aluminum electrode. Copolymer - solvent composition was varied from 1 wt% to 5 wt% in order to obtain sample thicknesses from 25 nm to 175 nm. Nonlinear permittivities up to ε_3 of poled and unpoled samples have been studied over temperature in heating and cooling cycles up to 120 °C i. e., above the Curie temperature. The polarization and its temperature dependence is derived from first and second order permittivities ε_1 and ε_2. Results offer a non-destructive readout of the polarization state. A non-switchable polarization is found which remains after heating the material above Curie temperature. This non-switchable polarization points from the bottom to the top electrode and is not influenced by the initial polarization direction.

DF 15.4 Thu 10:55 EB 107

Charge storing onto silicondioxide surfaces — •Bjoern Martin, Abhishek Rathi, and Herbert Kliem — Saarland University, Germany

The surface of silicondioxide/silicon structures is charged with the tip of a cantilever in contact mode by application of a voltage. Then, the surface potential is measured contactless using the Kelvin option of an atomic force microscope. On the position of the charged domain a potential difference in relation to the uncharged region is found.

It turns out that the height and the width of this potential difference depend on charging time, charging voltage, sample thickness, and doping of the silicon substrate. SiO_2/n-Si structures with thicknesses of about 10nm to 20nm contacted with negative voltages show the best charging behavior.

Additionally, a transient decay and a transient spread of the surface potential with a time constant of about 10h are observed. This time constant decreases with increasing humidity.

Due to the long-term stability and due to the possibility to reverse the sign of the deposited charges by charging in opposite direction an application of the system as surface charge memory device is thinkable.

It is remarkable and not yet fully understood why positive surface potentials indicating positive charges are found after charging with positive voltages.

DF 15.5 Thu 11:15 EB 107

Changes in microstructural and opto-electric properties of CrN films induced by vanadium ion implantation — Mirjana Novakovic[1], Agnes Traverse[2], Maja Popovic[1], Kun Zhang[3], •Klaus-Peter Lieb[3], and Natasha Bibic[1] — [1]VINČA Institute of Nuclear Sciences, 11001 Belgrade, Serbia — [2]Lab. Chimie Physique, Université Paris-Sud, 91405 Orsay, France — [3]II. Physikalisches Institut, Universität Göttingen, 37077 Göttingen, Germany

Transition-metal nitrides are known for their excellent tribological properties, making them important materials for protective hard coatings. In addition, CrN offers interesting thermoelectric and magnetic properties, correlated with a structural and magnetic phase transition at 273-286 K. The presence of additional transition-metals such as V or Mo plays an important role on their properties. We report on modifications of 280 nm CrN layers deposited on Si wafers via reactive sputtering and irradiated at room temperature with up to 2x1017 V-ions/cm2 at 80 keV. Rutherford backscattering spectroscopy (RBS), transmission electron microscopy (XTEM, HRTEM), and X-ray diffraction (XRD) were used to characterize changes in the structural properties. Their optical and electronic features were obtained by infrared spectroscopy in reflection mode and by electrical resistivity measurements. CrN was found to keep its cubic structure under the ion implantation; the initially partially non-metallic CrN layer displays metallic character, which could be related to Cr1-xVxN formation.

DF 16: Dielectric surfaces and interfaces

Time: Thursday 11:40–12:20 Location: EB 107

DF 16.1 Thu 11:40 EB 107

Resistive switching of Nb-doped $SrTiO_3$ single crystals — •Christian Rodenbücher, Krzysztof Szot, and Rainer Waser — Peter-Grünberg-Institut 7, Forschungszentrum Jülich, 52425 Jülich

The resistive switching effect in $SrTiO_3$ can be understood as an insulator to metal transition where a d-electron plays an important role which can be generated by creation of oxygen vacancies, electrodegradation or donor doping. In this talk we present the very surprising fact that Nb-doped $SrTiO_3$, although it is commonly regarded as a metallic material, can be switched. To clarify the nature of this phenomenon we investigated the crystallographic structure, the stoichiometry, the electronic structure and the transport by electrical measurements as well as by surface sensitive measurements like XPS, AFM and LEED which unquestionable reveal that switching occurs in a semiconducting surface layer which has greatly different properties than the metallic bulk. The stoichiometry and electronic structure of this surface layer can be dramatically altered by different preparation techniques like etching, leaching, heating in different atmospheres or Ar-bombardment. To get an insight in the nanoscopic origin of the switching, local conductivity AFM measurements were performed uncovering the highly local nature of the resistive switching which takes place in 10-30 nm big clusters which are present in the single crystal.

DF 16.2 Thu 12:00 EB 107

Water adsorption on $LiNbO_3$ Z-cut surfaces calculated from first principles — •Rebecca Hölscher, Simone Sanna, and Wolf Gero Schmidt — University of Paderborn

$LiNbO_3$ (LN) is a frequently used material for optical and acoustic applications due to its unusual but useful piezoelectric, pyroelectric, and photorefractive properties. As for other ferroelectric materials the surface reactivity can be changed by manipulating the polarization. This opens the possibility for the realization of molecular detectors and other devices[1]. Unfortunately only few data about the structure of the surface are available. Most studies do not refer to clean surfaces in UHV conditions, but are rather performed in ambient conditions, where the adsorption of foreign species like water will modify the the LN surface properties. Here we present ab initio calculations on the adsorption of H_2O molecules and thin water films on the positive (0001) and negative $(000\overline{1})$ surface of LN. The adsorption is modelled by means of density functional theory within the generalized gradient approximation[2,3]. The adsorption site and energy are determined as a function of the H_2O coverage. Different adsorption patterns are found depending on the surface polarity. The occuring water reconstruction is shown in phase diagrams as a function of temperature and pressure which reveal that at ambient conditions a H_2O film is present at the LN Z-cut.

[1] D. Li, M.H. Zhao, J. Garra, et al., Nature Materials ***7*** *(2008) 473. [2] W.G. Schmidt, M. Albrecht, S. Wippermann, S. Blankenburg, E. Rauls, et al., Phys. Rev. B* ***77*** *(2008), 035106. [3] S. Sanna, A.V. Gavrilenko, W.G. Schmidt, Phys. Stat. Sol. C* ***7*** *(2010) 145.*

DF 17: Focus Session: Alternative energies – Compensation of long- and short-term fluctuations (jointly with DY)

Organization: J. Peinke (Carl von Ossietzky Universität Oldenburg) and M. Diestelhorst (Martin-Luther-Universität Halle-Wittenberg)

Time: Thursday 15:00–18:10 Location: EB 107

Topical Talk DF 17.1 Thu 15:00 EB 107

Wind energy - Characterization and modeling of short-term fluctuations in incoming wind and power output — •Michael Hölling, Matthias Wächter, Allan Morales, Patrick Milan, and Joachim Peinke — ForWind - Center for Wind Energy Research, Institute of Physics, University of Oldenburg

One inherent characteristic of turbulent atmospheric wind fields is their correlation in time and space, which results in intermittent behavior of velocity increments on a wide range from very small to very large scales. Wind energy converters work in this highly intermittent environment and transfer these fluctuations to the generator and the power output, respectively. With a significantly increased wind power production in the future, there is a need to better understand the interaction of turbulent wind fields with wind turbines. We present methods to describe and model these intermittent characteristics of atmospheric flows and power output of wind turbines using stochastic analysis. Data from wind tunnel experiments on blade segments with respect to lift forces under turbulent wind conditions show dynamic stall like behavior with an increased maximum lift force shifted to higher angles of attack compared to laminar inflow conditions. In addition an increase in the standard deviation in the acting lift forces is observed, which leads to dynamic changes in loads, that have to be accounted for e.g. in the design process of the wind turbine. Also the power output from wind turbines shows intermittent behavior resulting from the turbulent wind fields. The presented methods can help to describe and predict power fluctuations and to make the machines last longer.

Topical Talk DF 17.2 Thu 15:30 EB 107

Fluktuationen in der Stromerzeugung aus erneuerbarer Energien: Ihre Charakterisierung und Möglichkeiten ihrer Kompensation — •Detlev Heinemann — AG Energiemeteorologie, Institut für Physik, Universität Oldenburg

Die Beitrag der erneuerbaren Energien aus Wind und Solarstrahlung an der deutschen Stromversorgung nähert sich der 20%-Marke. Damit sind erhebliche und nur teilweise vorhersagbare Schwankungen der Erzeugung verbunden und es wird z.B. zunehmend der Bedarf an Systemunterstützung z.B. durch Speicherung diskutiert. Noch wenig bekannt ist, wie weit dieser Speicherbedarf durch Ausnutzung von vorhandenen Ausgleichseffekten und durch eine intelligente Steuerung des Verhaltens der Komponenten im Stromnetz ('Smart Grid') unter Einbeziehung einer präziseren Charakterisierung der Fluktuationen reduziert werden kann.

Der Beitrag charakterisiert - ausgehend von einer Phänomenologie der beobachteten Ereignisse - die für die Energieträger Wind und Solarstrahlung wesentlichen Fluktuationen. Dabei werden die unterschiedlichen zeitlichen und räumlichen Skalen der Fluktuationen betrachtet und ebenfalls räumliche Korrelationen der zeitlichen Schwankungen untersucht. Die Beeinflussung der effektiven Stromerzeugungs-Kapazität aus Wind- und Solarenergie durch diese statistischen Effekte wird diskutiert. Abschliessend werden aktuelle Ansätze eines Ausgleichs dieser Fluktuationen sowohl durch technische Massnahmen als auch durch den Einsatz intelligenter Verfahren vorgestellt.

Topical Talk DF 17.3 Thu 16:00 EB 107

Glasses and glass ceramics as dielectrics for high power capacitors. — •Martin Letz — Schott AG, Mainz, Germany

Temperature stable, reliable and long lasting capacitors are a key component for high power electronics enabling large amount of fluctuating energy sources in the public electricity grid. Since many decades inorganic materials are known as excellent dielectrics. Among these thin foils made from alkaline free special glass are known for their very good homogeneity and excellent surface roughness. Such glass foils can reach dielectric breakdown strengths of 690 kV/mm (measured at 0.025 mm thickness) and more. Due to their excellent thermal stability they can be used for temperatures up to 500 °C as dielectrics in capacitors. A further class of materials are glass ceramics obtained via a true homogeneous glassy phase. Here it is possible to crystallize out ferroelectric phases like BaTiO3 in form of nano crystallites leading to high dielectric constants. Obtained from a true glassy phase such glass ceramics are free of pores and reach dielectric breakdown strengths of

40kV/mm (measured at 0.2 mm thickness). The current development for such glasses and glass ceramics is presented which shows the possibility for obtaining high power capacitors which exceed the energy storage capacity of todays high power capacitor solutions by more than one order of magnitude.

DF 17.4 Thu 16:30 EB 107

The dielectric AC and DC characterisation of composite capacitors for energy storage — •Sebastian Lemm[1], Wolfram Münchgesang[1], Martin Diestelhorst[1], Mandy Zenkner[2], Thomas Grossmann[2], Alexandra Buchsteiner[3], Horst Beige[1], Stefan G. Ebbinghaus[2], and Hartmut S. Leipner[3] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Institut für Chemie, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [3]Interdisziplinäres Zentrum für Materialwissenschaften , Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

Today, rechargeable batteries are mostly used for energy storage. An alternative to the electrochemical storage process in batteries are capacitors with a high energy density and a long carrier storage time. For the design and development of such capacitors the default dielectric AC characterisation method for capacitors is inadequate because the energy storage process operates under DC conditions. We present a measurement procedure which includes DC and AC characterisation using the example of composite capacitors consisting of barium titanate nanoparticles embedded in a matrix material. Furthermore we show the differences between the measurement methods and the problems of analysing such capacitors.

DF 17.5 Thu 16:50 EB 107

Permittivity, energy density and carrier storage time of film composite capacitors — •Wolfram Münchgesang[1], Sebastian Lemm[1], Martin Diestelhorst[1], Claudia Ehrhardt[2], Jens Glenneberg[3], Alexandra Buchsteiner[3], Horst Beige[1], Stefan G. Ebbinghaus[2], and Hartmut S. Leipner[3] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Institut für Chemie, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [3]Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

Thin film composite capacitors are a possible alternative for batteries as energy storage. Their anticipated advantages are short charging and discharging times, a long life cycle, higher energy density and lower temperature dependency. We tested this predicted behaviour of such film composite capacitors under DC and AC conditions. The thin film composites based on nanoparticles of barium titanate which are embedded in a polymeric organic matrix and surface-modified by surfactants.

Topical Talk DF 17.6 Thu 17:10 EB 107

High Tc Superconducting Energy Storage Systems — •Frank Werfel — Adelwitz Technologiezentrum GmbH (ATZ), Arzberg-Adelwitz, Germany

Electric energy is basic to heat and light our homes, to power our businesses and to transport people and goods. Powerful storage techniques like SMES, Flywheel, Super Capacitor, and Redox - Flow batteries are needed to increase the overall efficiency, stability and quality of electrical grids. High-Tc superconductors (HTS) possess superior physical and technical properties and can contribute in reducing the dissipation and losses in electric machines as motors and generators, in electric grids and transportation. The renewable energy sources as solar, wind energy and biomass will require energy storage systems even more as a key technology. We survey the physics and the technology status of superconducting flywheel energy storage (FESS) and magnetic energy storage systems (SMES) for their potential of large-scale commercialization. We report about a 10 kWh / 250 kW flywheel with magnetic stabilization of the rotor. The progress of HTS conductor science and technological engineering are basic for larger SMES developments. The performance of superconducting storage systems is reviewed and compared. We conclude that a broad range of intensive research and development in energy storage is urgently needed to produce technological options that can allow both climate stabilization and economic development.

Topical Talk DF 17.7 Thu 17:40 EB 107

The transmission of high-power microwaves via dielectric diamond windows: Design, qualification and first steps towards a broadband diamond window in the range of 30GHz to several THz for actual and future fusion devices — •Theo Scherer and Dirk Strauss — Karlsruhe Institute of Technology KIT; D-76021 Karlsruhe

The development of artificial diamond disks fabricated by special RF CVD processes lead to a new generation of dielectric high power millimetre wave windows with extremely low absorption and scattering losses for high power transmission. The quality of diamond as a window material is further given by its well known excellent mechanical properties and extremely high thermal conductivity. The growth process of the diamond disks is based on chemical vapour deposition (CVD) with micro/nano diamond nuclei. The transmission losses of the disk are caused by graphite formation mainly at the surface of the disk but also on the grain boundaries. RAYLEIGH scattering limits the value of loss tangent in bulk. A high quality measurement of the disk surface and bulk properties using spherical and hemispherical resonators is presented for frequencies from 90 up to 170 GHz.

The state of the art windows used in high power electron cyclotron heating and current drive (ECRH&CD) for large fusion devices such as ITER consist of a disk perpendicular to the millimetre wave beam propagation. As reflection have to be kept on a minimal level, the window thickness limits the allowed frequencies to a limited set defined by multiples of lambda/2 in the dielectric matter.

DF 18: Resistive switching I (jointly with DS, KR, HL)

Time: Friday 9:30–10:45 Location: H 0111

DF 18.1 Fri 9:30 H 0111

Ab-initio studies of metal-insulator transitions in defective perovskites — •Gustav Bihlmayer and Kourosh Rahmanizadeh — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Resistive switching in perovskite materials can be triggered by a variety of external stimuli, like electric fields or oxygen partial pressure. While the role of oxygen defects for the electronic transport is in many cases established, the nature of the metal-insulator transition has still to be explored. Density functional theory calculations including strong correlation effects on a model level can help to gain an understanding here.

We investigate the transition between an insulating state of a correlated, localized level and a partially filled conductive band as function of electron concentration. The band filling can be controlled in a chemical way or via electric fields. A ferroelectric polarization can screen or enhance the effects at the boundaries of a ferroelectric material. We study the localization of defect states in model systems of structurally simple perovskites like $SrTiO_3$ or $PbTiO_3$ to gain a coherent picture of the conductive states that are manipulated in the resistive switching process.

Financial support of the EU grant NMP3-LA-2010-246102 (IFOX) is gratefully acknowledged.

DF 18.2 Fri 9:45 H 0111

Elucidation of the resistive switching in $SrTiO_3$ MIM-structures by μXANES — •Christian Lenser[1,2], Alexei Kuzmin[3], Alexandr Kalinko[3], Juris Purans[3], Rainer Waser[1,2,4], and Regina Dittmann[1,2] — [1]Peter Grünberg Institut 7, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich-Aachen Research Alliance, Section Fundamentals of Future Information Technology (JARA-FIT), Germany — [3]Institute of Solid State Physics, University of Latvia, Kengaraga Street 8, LV- 1063 Riga, Latvia — [4]Institut für Werkstoffe der Elektrotechnik, RWTH Aachen, 52056 Aachen, Germany

The resistive switching effect in Fe-doped $SrTiO_3$ thin films is investigated on 100 μm^2 metal-insulator-metal (MIM) structures by chemical mapping in the μm regime. X-ray absorption fine structure (XAFS)

- measured at beamline ID03, ESRF - with a x-ray beam focused to several μm provides information about the absorption fine structure modulations at the Fe K-edge. The increase of pre-edge intensity characteristic of oxygen vacancies in the first coordination shell of the transition metal dopant shows the films to be highly oxygen deficient after growth. In addition to an increase of the Fe-$V_O^{\bullet\bullet}$ concentration over the whole electrode area after electroforming, μm-sized mapping of a MIM-structure reveals the location of the conducting filament by a strong local change in the absorption edge, which is localized to a size of the order of 1 μm. The change of the absorption characteristics is interpreted with full multiple-scattering XANES simulations, suggesting oxygen vacancy clustering around Fe as the likely explanation.

DF 18.3 Fri 10:00 H 0111

A ferroelectric switchable tunnel junction: $KNbO_3/SrTiO_3$ — •Kourosh Rahmanizadeh, Gustav Bihlmayer, Daniel Wortmann, and Stefan Blügel — Peter Grünberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The properties of thin oxide films and multilayers are strongly influenced by defects and, therefore, can be controllably tuned by the defect concentration at the interface. For example, due to the charge discontinuity at the $SrTiO_3$/KO-$KNbO_3$-NbO_2/$SrTiO_3$ interface only one direction of polarization in $KNbO_3$ film is stable. A switchable polarization in $KNbO_3$ can be realized by creating (oxygen) defects at the interfaces.

We carried out density functional theory (DFT) calculations based on the full potential linearized augmented planewave (FLAPW) method as implemented in the FLEUR code [1] for studying the polar interface $SrTiO_3/KNbO_3$ and a $SrRuO_3/SrTiO_3/KNbO_3$ tunnel junction. The electronic transport properties of the switchable multiferroic $SrRuO_3/SrTiO_3$/KO-$KNbO_3$-$NbO_3/SrTiO_3/SrRuO_3$ heterostructure have been investigated using an embedded Green-function approach [2]. A strong dependence of the (magneto electric) transport properties on the polarization is observed. The work was conducted under the auspices of the IFOX consortia under grant agreement NMP3-LA-2010-246102.

[1] http://www.flapw.de
[2] D. Wortmann, H. Ishida, and S. Blügel, PRB **66**, 075113 (2002)

DF 18.4 Fri 10:15 H 0111

Resistive switching in different forming states of Ti/$Pr_{0.48}Ca_{0.52}MnO_3$ junctions — •Chanwoo Park[1], Anja Herpers[1], Rainer Bruchhaus[1], Johan Verbeeck[2], Ricardo Egoavil[2], Francesco Borgatti[3], Giancarlo Panaccione[4], Francesco Offi[5], and Regina Dittmann[1] — [1]PGI-7, FZ Jülich — [2]EMAT, University of Antwerp, Belgium — [3]ISMN-CNR, Bologna, Italy — [4]Laboratorio Nazionale TASC-INFM-CNR, Trieste, Italy — [5]CNISM and Dipartimento di Fisica, Università Roma Tre, Rome, Italy

We investigated the resistive switching (RS) characteristics of Ti/$Pr_{0.48}Ca_{0.52}MnO_3$ (PCMO) junctions. RS characteristics were observed after a first forming (1stF) procedure, which changes the initial resistance state to a high resistance state (HRS) which shows a clear area dependence. By performing Hard X-ray Photoelectron Spectroscopy for different resistive states, we found a change of the Ti2p peak intensity after the 1stF which is associated with the formation of TiO_2 at the interface. Moreover, the shape and position of the Mn2p peak hints on the reduction of Mn. The formation of TiO_x at the Ti/PCMO interface after the 1stF was confirmed by cross-sectional Transmission Electron Microscope investigations. The results indicate that the 1stF step is related to a redox process at the Ti/PCMO interface. Moreover, we were able to perform a second forming step which changes the HRS to the low resistance. The area dependence disappeared after the second forming. This implies that conducting filaments might form at the Ti/PCMO interface.

DF 18.5 Fri 10:30 H 0111

Remanent resistance changes in metal- PrCaMnO-metal sandwich structures — •Malte Scherff, Bjoern Meyer, Julius Scholz, Joerg Hoffmann, and Christian Jooss — Institute of Materials Physics, University of Goettingen, Germany

The non-volatile electric pulse induced resistance change (EPIR) seems to be a rather common feature of oxides sandwiched by electrodes. However, microscopic mechanisms are discussed controversially. We present electrical transport measurements of sputtered $Pr_{0.7}Ca_{0.3}MnO_3$ films sandwiched by metallic electrodes with variation of electrode materials, device geometry and PCMO deposition parameters. Cross-plane transport measurements have been performed as function of temperature and magnetic field. Specifically, the transition from dynamic resistance changes due to non-linear transport to remanent switching is analyzed. By analyzing changes of magnetoresistance at low temperatures in different resistance states we aim for separation between interface and film contributions to switching. Comparing switching behavior in symmetric and asymmetric electrode configuration allows for identification of the active, single interface in the switching process and the origin of an observed switching polarity inversion[1]. The influence of excitation field and power on the switching characteristics of different noble metal electrodes is discussed. Samples from macroscopic devices and in situ stimulated sandwich structures were studied in a transmission electron microscope in order to investigate the induced structural, chemical and electronic changes. [1] M. Scherff et al, J.Appl.Phys. 110, 043718 (2011)

DF 19: Resistive switching II (jointly with DS, KR, HL)

Time: Friday 11:00–12:30 Location: H 0111

DF 19.1 Fri 11:00 H 0111

Resistive switching mechanism of Ti/HfO_2/TiN RRAM cells studied by nondestructive hard x-ray photoelectron spectroscopy — •Małgorzata Sowińska[1], Thomas Bertaud[1], Damian Walczyk[1], Christian Walczyk[1], Sebastian Thiess[2], Wolfgang Drube[2], and Thomas Schroeder[1] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt/Oder, Germany — [2]DESY, Notkestrasse 85, 22607 Hamburg, Germany

A variety of different metal-insulator-metal (MIM) multilayered structures reveal reversible changes in resistance upon applying bias voltages across the layers. The physical mechanism of this resistive switching effect in such MIM cells is mostly unknown up to nowadays, although different models depending on the switching behaviour (unipolar or bipolar) and the conducting path type (filamentary or interface) have been proposed. In order to identify whether the resistance variation in the Ti/HfO_2/TiN system is related to local changes in the chemistry or to charge distribution we performed ex-situ and in-situ hard x-ray photoelectron spectroscopy (HAXPES) studies. This technique is well suited for investigating the buried interface of our resistive random access memory (RRAM) cell in a nondestructive way. In result, spectral differences observed between as-deposited and electrically switched devices lead us to the conclusion that the Ti/HfO_2 interface was modified, which can be associated with an interface-type model. Furthermore, we have also better revealed the impact of the current compliance on the HAXPES spectra of our device.

DF 19.2 Fri 11:15 H 0111

Pulse-induced resistive switching of CMOS embedded HfO_2-based 1T1R cells — •damian walczyk, christian walczyk, thomas bertaud, małgorzata sowińska, mindaugas lukosius, steffen kubotsch, thomas schroeder, and christian wenger — IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany.

Low-cost embedded nonvolatile memories (eNVMs) with high-density, high-speed, and low-power are of interest for many different system applications in Si-based CMOS technologies, including consumer electronics, high-end and mobile computing, various sensor and medical health care devices. The rising importance of embedded NVM technologies in recent years has pushed Resistance change Random Access Memory (RRAM) into the spotlight. However, despite numerous integration efforts, the driving mechanism for the resistive switching effect of HfO_2-based RRAM is still under debate [1]. Progress in the development has mainly been delayed due to the lack of control over the switching parameters. To achieve an application relevant endurance, the capability to control the resistance by an access device is addressed in this talk. Moreover, this work considers the pulse-induced resistive switching of memory cells with an area down to $1 \times 1\ \mu m^2$. It is

observed that the pulse width range for the set process is between 60 ns and 80 ns while the reset encompasses a pulse width range of 10-30 μs. Due to the intrinsic current compliance of the access transistor, low set currents of 10 μA and reset currents of 1 μA are obtained.

[1] C. Walczyk et al., IEEE Trans. Electron. Devices, vol. 58, no. 9, pp. 3124-3131 (2011).

DF 19.3 Fri 11:30 H 0111

Resistive switching on HfO_2-based metal-insulator-metal structures: effects of the top metal electrode and the oxygen partial pressure — •Thomas Bertaud[1], Damian Walczyk[1], Christian Walczyk[1], Steffen Kubotsch[1], Malgorzata Sowinska[1], Thomas Schroeder[1], Christophe Vallée[2], Vincent Jousseaume[3], and Christian Wenger[1] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt Oder, Germany — [2]LTM Université Joseph Fourier, 17 Rue des Martyrs 38054 Grenoble, France — [3]CEA-LETI Minatec, 17 Rue des Martyrs 38054 Grenoble, France

Embedded nonvolatile memories (eNVM) are attractive for a growing number of applications. One promising candidate for next-generation eNVM is based on the electrically switchable resistance change between a high and a low resistive state of a metal-insulator-metal (MIM) structure, called resistance random access memory (RRAM). Due to the cost effectivity and BEOL compatibility with (Bi)CMOS technologies, this approach is highly attractive. In this talk, the resistive switching on HfO_2/bottom TiN based devices will be demonstrated. The work is focused on the impact of the top metal electrode on the switching behavior of the RRAM devices: Al, Hf and Ti (reactive non-blocking), and Cu, Pt and Au (non-reactive blocking) are used and lead to bipolar or unipolar switching, respectively [1]. The current and capacitance characteristics of the MIM diodes are studied by voltage sweeps and retention measurements under different gas ambient in order to highlight the effect of the oxygen partial pressure for a better understanding of the mechanism. [1] T. Bertaud et al., Thin Solid Films (2011).

DF 19.4 Fri 11:45 H 0111

A model for a non-volatile memory material: First principles study of Cu diffusion in α-cristobalite and α-quartz — •Martin Zelený[1], Jozsef Hegedüs[1], Adam. S. Foster[2], David. A. Drabold[3], Stephen. R. Elliott[4], and Risto. M. Nieminen[1] — [1]COMP/Dept. of Applied Physics, Aalto University School of Science, Espoo, Finland — [2]Dept. of Physics, Tampere University of Technology, Tampere, Finland — [3]Dept. of Physics and Astronomy, Ohio University, Athens, USA — [4]Dept. of Chemistry, University of Cambridge, Cambridge, UK

The switching mechanism of a new type of non-volatile memories can be based on electrochemical metallization occurring due to the migration of Ag or Cu ions in oxide glasses as for example SiO_2. In order to clarify this mechanism, we have performed simulations of Cu diffusion in the different modifications of SiO_2. All calculations in our study were carried out based on first-principles density-functional theory using the Vienna Ab initio Simulation Package (VASP).

We present a total-energy calculation of the barrier along a diffusion path of Cu between two equivalent interstitial positions in α-cristobalite and α-quartz. Our results for α-cristobalite show that the shape of the path strongly depends on the charge of the system, but the height of the migration barrier stays between 0.15-0.2 eV. On the other hand, the height of the barrier in α-quartz varies between 0.1 and 0.6 eV and depends on the directions of Cu motion. We also present results of molecular dynamics simulations of the drift of a Cu atom driven by an external electric field.

DF 19.5 Fri 12:00 H 0111

Transient Processes in Response to Electronic Excitation of Phase Change Materials — •Martin Salinga and Martin Wimmer — 1. Institut of Physics, RWTH Aachen University, Germany

In recent years a strong interest in phase change materials has been aroused by their potential for being utilized as the core element of a promising novel electronic memory technology. For such an application it is crucial to understand the characteristic switching mechanisms. Especially the electronic properties of the amorphous phase are of paramount importance. Thus, the strong non-linearity in the current-voltage-dependence of the amorphous phase, often referred to as threshold-switching, has drawn much attention.

In this work the transient current response of vertical Ge2Sb2Te5 devices to controlled voltage excitations is experimentally studied down to a time-scale of a few nanoseconds and analyzed with a particular focus on the delay-time before threshold switching and its dependence on the applied voltage. The results are compared to both experimental and theoretical studies in the literature and their implications for this field of research are discussed.

DF 19.6 Fri 12:15 H 0111

Nonvolatile resistive switching in Au/BiFeO3 rectifying junction — •Yao Shuai[1,2], Chuangui Wu[2], Wanli Zhang[2], Shengqiang Zhou[1], Danilo Bürger[1], Stefan Slesazeck[3], Thomas Mikolajick[3], Manfred Helm[1], and Heidemarie Schmidt[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, P. O. Box 510119, Dresden 01314, Germany — [2]State Key Laboratory of Electronic Thin Films and Integrated Devices, Chengdu, China — [3]Namlab gGmbH, Nöthnitzer Strasse 64, 01187 Dresden, Germany

BiFeO3 thin films have been grown on Pt/Ti/SiO2/Si substrates with pulsed laser deposition. RF sputtered Au has been used for the top electrode. The transport properties of the BiFeO3 thin films have been previously demonstrated to be sensitive to the interface [1]. In the present work, an interface-related resistive switching behavior with large switching ratio up to 4500 has been observed in the Au/BiFeO3/Pt structure [2]. The different polarities of the external voltage induce an electron trapping or detrapping process, and consequently change the depletion layer width below the Au Schottky contact, which is revealed by capacitance-voltage measurements and by long-term low/high resistance state capacitance transient measurements at zero bias [3]. [1] Y. Shuai et al., Appl. Phys. Lett., 98, 232901 (2011). [2] Y. Shuai et al., Appl. Phys. Express. 4, 095802 (2011). [3] Y. Shuai et al., J. Appl. Phys. 109, 124117 (2011).