Crystallography Division
Fachgruppe Kristallographie (KR)

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Overview of Invited Talks and Sessions

(lecture rooms E 124, EMH 225 and H 0105; Poster A and E)

Invited Talks

KR 6.1	Tue	9:30–10:00	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, Siegfried Däbritz, Enrico Langer, Jürgen Bauch, Andreas Danilewsky, Peter Paufler
KR 10.1	Thu	9:30–10:00	E 124	**On polytypism in III-V nanowires** — •Friedhelm Bechstedt, Abderrezak Belabbes, Christian Panse, Jürgen Furthmüller, Dominik Kriegner, Julian Stangl

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

KR 1.1–1.5	Mon	15:00–17:30	H 0105	**SYXD: 100 years of X-ray diffraction: from the Laue experiment to new frontiers (Joint Symposium KR, BP, CPP, DF, MA, MM, GP – Organization: Wiehl, Grübel, Rädler)**
KR 2.1–2.11	Mon	9:30–12:45	EB 301	**Joint Session "Multiferroics I - Junctions and Thin Films / Magnetoelectric Coupling" (MA jointly with DF, DS, KR, TT), Organization: Manfred Fiebig (ETH Zürich)**
KR 3.1–3.12	Mon	15:00–18:30	EB 301	**Joint Session "Multiferroics II - Hexagonal Manganites / Incommensurate Multiferroics" (MA jointly with DF, DS, KR, TT)**
KR 4.1–4.12	Tue	9:30–12:45	EB 301	**Joint Session "Multiferroics III - Strain / New Routes towards Multiferroicity" (MA jointly with DF, DS, KR, TT)**
KR 5.1–5.90	Tue	12:15–15:15	Poster A	**Poster I – including Multiferroics (MA with DF, DS, KR, TT)**
KR 6.1–6.11	Tue	9:30–12:45	EMH 225	**100 years since the Laue experiment: Topical aspects of diffraction and scattering (Joint Session KR, BP, DF, GP, MA, MI, MM; related to SYXD)**
KR 7.1–7.6	Wed	9:30–12:30	BH 243	**Joint Session "Soft X-ray Resonant Scattering for Complex Structural and Magnetic Investigations" (MA jointly with KR), Organization: Eberhard Goering (MPI-IS Stuttgart)**
KR 8.1–8.4	Wed	15:00–17:30	Poster E	**Poster – 100 years since the Laue experiment: Topical aspects of diffraction and scattering (Joint Session KR, BP, DF, GP, MA, MI, MM; related SYXD)**
KR 9.1–9.2	Wed	15:00–17:30	Poster E	**Poster – Crystallography in Nanoscience**
KR 10.1–10.7	Thu	9:30–12:00	E 124	**Crystallography in Nanoscience**
KR 11.1–11.5	Thu	15:00–17:30	H 0105	**SYRS: Symposium Resistive Switching (joint symposium DS, DF, KR, HL – Organizers: Gemming, Dittmann)**
KR 12	Thu	17:45–18:30	E 124	**Mitgliederversammlung FG Kristallographie**

Annual General Meeting of the Crystallography Division

Donnerstag 17:45–18:30 E 124

- Bericht
- Tagungsplanung 2013
- Verschiedenes

KR 1: SYXD: 100 years of X-ray diffraction: from the Laue experiment to new frontiers (Joint Symposium KR, BP, CPP, DF, MA, MM, GP – Organization: Wiehl, Grübel, Rädler)

Time: Monday 15:00–17:30 Location: H 0105

Invited Talk KR 1.1 Mon 15:00 H 0105
Disputed discovery: The beginnings of X-ray diffraction in crystals — •Michael Eckert — Deutsches Museum, Forschungsinstitut, Museumsinsel 1, D-80538 München

The discovery of X-ray diffraction in crystals was based on misconceptions about the nature of X-rays. The background of "Laue's discovery" and its early repercussions are described from the perspective of contemporary views in 1912. The riddle concerned the origin of the monochromacy observed in the Laue spots.

Invited Talk KR 1.2 Mon 15:30 H 0105
Why are quasicrystals quasiperiodic? — •Walter Steurer — Laboratorium für Kristallographie, ETH Zürich, Wolfgang-Pauli-Strasse 10, 8093 Zürich, Schweiz

It took more than two years until Dan Shechtman could publish his finding of a rapidly solidified Al-Mn phase with sharp Bragg reflections and icosahedral point group symmetry. His results were not accepted, initially, since they seemed to contradict fundamental laws of crystallography. A further twenty-seven years had to pass by until his discovery of quasicrystals was honoured by the Nobel Prize in 2011. This discovery was fundamental because quasiperiodic order represents a novel equilibrium state of solid matter fundamentally different from the common periodic one.

At present, stable quasicrystals have been found in more than fifty binary and ternary intermetallic systems. They show mostly decagonal or icosahedral diffraction symmetry contrary to soft quasicrystals. These are mainly qasiperiodic structures resulting from the self-assembly of either micelles in a liquid or of terpolymers with dodecagonal symmetry. The so far most promising applications of quasiperiodic structures seem to be in the field of photonic and phononic crystals.

The focus of the talk will be on the driving forces for the formation and stablization of quasiperiodic structures.

Invited Talk KR 1.3 Mon 16:00 H 0105
Coherent Diffraction Imaging with Free-Eletron Lasers — •Massimo Altarelli — European XFEL GmbH, 22607 Hamburg

One hundred years after the discovery of x-ray diffraction from crystals, spatially coherent, ultra-brilliant and ultra-short pulses of x-ray radiation from free electron lasers (FEL's) open the way to structure solution without the hurdle of crystallization. Biological objects such as cells, viruses, possibly down to individual macromolecules and to atomic resolution, and individual nanostructures in material sciences are eligible for these novel studies. An overview of the x-ray FEL sources and their basic physical principles and properties, of the strategies for sample handling and data collection and a glimpse of the necessary algorithms to phase the diffraction patterns are given. Example of results from the soft x-ray FLASH source in Hamburg and from the Linac Coherent Light Source in Stanford are illustrated. The perspectives and the challenges of the high repetition rate (up to 27 000 pulses/s) of the European XFEL, under construction in the Hamburg region, are also briefly discussed

Invited Talk KR 1.4 Mon 16:30 H 0105
X-ray free-electron lasers - emerging opportunities for structural biology — •Ilme Schlichting — Max Planck Institute for Medical Research, Heidelberg, Germany

X-ray crystallography is a mature yet still advancing method for structure determination of molecules with any molecular weight. Facilitated greatly by synchrotron X-ray sources, the method is limited only by the quality and size of the crystals and by radiation damage. Free-electron lasers (FELs) provide orders of magnitude brighter and shorter X-ray pulses than conventional synchrotron sources. It has been proposed that radiation damage, which limits the high resolution imaging of soft condensed matter, can be "outrun' by using ultrafast and extremely intense X-ray pulses that pass the sample before the onset of significant radiation damage [1]. Thus, one of the most promising scientific applications of XFELs is in sub-nanometer resolution imaging of biological objects, including viruses, macromolecular assemblies, and nanocrystals. The concept of "diffraction-before-destruction" has been demonstrated recently at the Linac Coherent Light Source (LCLS) [2], the first operational hard X-ray FEL, for protein micro- and nanocrystals [3] and single mimivirus particles [4]. These experiments and recent developments and progress will be presented.

[1]. Neutze et al., Nature 406, 752-757 (2000). [2]. Emma, Nature Photonics 4, 641-647 (2010). [3]. Chapman et al., Nature 470, 73-77 (2011). [4]. Seibert et al., Nature 470, 78-81 (2011).

Invited Talk KR 1.5 Mon 17:00 H 0105
Structure analysis by x-ray diffraction and x-ray imaging: beyond crystals, beyond averages, and beyond modeling — •Tim Salditt — Georg-August-Universität Göttingen, Institut für Röntgenphysik, Friedrich-Hund-Platz 1, 37077 Göttingen

Classical x-ray diffraction has been based on three constraints: (i) averages over macroscopic accumulation time and sample sizes, which are many orders of magnitude larger than the structures to be resolved; (ii) homeogeneous "well ordered" samples which are - if not crystalline - characterized by well-defined correlation functions; (iii) data analysis by fitting to modeled diffraction data. However, many condensed matter problems, in particular in functional materials, soft matter and biomolecular samples, address non-equilibrium states with competing length scales, hierachical structures, and intrinsic dynamics. Progress in x-ray sources and optics has helped to meet these challenges. Conceptually often still close to the Laue experiment, far-field diffraction data can now be collected in controllable field of vies, with highly focused beams reaching the 10 nm range. Biomolecular diffraction signals can be recorded from hierachical structures such as a biological cells. Perhaps most importantly, fully coherent illumination enables data inversion without prohibitive model building. How these advances serve science, will be illustrated by examples in neuro-biophysics. We present experiments addressing different structural levels and bridging length scales, from proteins and lipid assemblies up to a complete organelle such as the synaptic vesicle, from an isolated axon up to an unsliced nerve, from tissue slice to the sensory organ.

KR 2: Joint Session "Multiferroics I - Junctions and Thin Films / Magnetoelectric Coupling" (MA jointly with DF, DS, KR, TT), Organization: Manfred Fiebig (ETH Zürich)

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

Topical Talk KR 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.

KR 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.

KR 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)

KR 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.

KR 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

KR 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.

KR 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.

KR 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.

KR 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 Li$M$$PO_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 unsual, photosensitive temperature dependence which is discussed in detail.

- Work supported by the SFB 608 of the DFG.

KR 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.

KR 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.

KR 3: Joint Session "Multiferroics II - Hexagonal Manganites / Incommensurate Multiferroics" (MA jointly with DF, DS, KR, TT)

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

Invited Talk KR 3.1 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.

KR 3.2 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).

KR 3.3 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.

KR 3.4 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.

KR 3.5 Mon 16:15 EB 301

Sinusoidal electromagnon in $R\mathbf{MnO_3}$: 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.

KR 3.6 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.

KR 3.7 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

KR 3.8 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.

KR 3.9 Mon 17:30 EB 301

A further step of understanding the complex magnetic order in magnetoelectric $\mathbf{Co_3TeO_6}$ — •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.

KR 3.10 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.

KR 3.11 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).

KR 3.12 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 $400\,\mu C/m^2$ 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)

KR 4: Joint Session "Multiferroics III - Strain / New Routes towards Multiferroicity" (MA jointly with DF, DS, KR, TT)

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

KR 4.1 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.

KR 4.2 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.

KR 4.3 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) re-

sponses 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.

KR 4.4 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 %.

KR 4.5 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.

KR 4.6 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 ($R\overline{3}c$), 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).

KR 4.7 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).

KR 4.8 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

KR 4.9 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).

KR 4.10 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).

KR 4.11 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.

KR 4.12 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)

KR 5: Poster I – including Multiferroics (MA with DF, DS, KR, TT)

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

KR 5.1 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.

KR 5.2 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.

KR 5.3 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.

KR 5.4 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.

KR 5.5 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.

KR 5.6 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.

KR 5.7 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.

KR 5.8 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.

KR 5.9 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.

KR 5.10 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.

KR 5.11 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.

KR 5.12 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.

KR 5.13 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 %.

KR 5.14 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).

KR 5.15 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.

KR 5.16 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.

KR 5.17 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.

KR 5.18 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 ferromagnetic 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 $T_{\text{ann}} \approx 700°$ 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).

KR 5.19 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.

KR 5.20 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.

KR 5.21 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.

KR 5.22 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).

KR 5.23 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).

KR 5.24 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.

KR 5.25 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

KR 5.26 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)

KR 5.27 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.

KR 5.28 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.

KR 5.29 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)

KR 5.30 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.

KR 5.31 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.

KR 5.32 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.

KR 5.33 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.

KR 5.34 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.

KR 5.35 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 cy-

cloidal 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)

KR 5.36 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

KR 5.37 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).

KR 5.38 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.

KR 5.39 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.

KR 5.40 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.

KR 5.41 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.

KR 5.42 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).

KR 5.43 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.

KR 5.44 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.

KR 5.45 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.

KR 5.46 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.

KR 5.47 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)

KR 5.48 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

KR 5.49 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.

KR 5.50 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)

KR 5.51 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).

KR 5.52 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.

KR 5.53 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.

KR 5.54 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 $Fe_{76}Gd_{24}$ 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.

KR 5.55 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.

KR 5.56 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.

KR 5.57 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.

KR 5.58 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.

KR 5.59 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.

KR 5.60 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.

KR 5.61 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).

KR 5.62 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.

KR 5.63 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 (NRLMOL/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

KR 5.64 Tue 12:15 Poster A

Optimization of spin-valve structures for spin-pumping experiments — •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)

KR 5.65 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)

KR 5.66 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.

KR 5.67 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).

KR 5.68 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

KR 5.69 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.

KR 5.70 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.

KR 5.71 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.

KR 5.72 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.

KR 5.73 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)

KR 5.74 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.

KR 5.75 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)

KR 5.76 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)

KR 5.77 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.

KR 5.78 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

KR 5.79 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)

KR 5.80 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.

KR 5.81 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.

KR 5.82 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

KR 5.83 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.

KR 5.84 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.

KR 5.85 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.

KR 5.86 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).

KR 5.87 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.

KR 5.88 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.

KR 5.89 Tue 12:15 Poster A

Broadband Electron Spin Resonance Experiments using superconducting 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.

KR 5.90 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)

KR 6: 100 years since the Laue experiment: Topical aspects of diffraction and scattering (Joint Session KR, BP, DF, GP, MA, MI, MM; related to SYXD)

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

Invited Talk KR 6.1 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.

KR 6.2 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)

KR 6.3 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).

KR 6.4 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.

KR 6.5 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.

KR 6.6 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

KR 6.7 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.

KR 6.8 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)

KR 6.9 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.

KR 6.10 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.

KR 6.11 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.

KR 7: Joint Session "Soft X-ray Resonant Scattering for Complex Structural and Magnetic Investigations" (MA jointly with KR), Organization: Eberhard Goering (MPI-IS Stuttgart)

Time: Wednesday 9:30–12:30 Location: BH 243

Invited Talk KR 7.1 Wed 9:30 BH 243

Soft X-ray Resonant Magnetic Reflectometry of Ferromagnet/Antiferromagnet Interfaces - Probing the Origin of Exchange Bias — •Sebastian Brück[1], Gisela Schütz[2], Kannan M. Krishnan[3], and Eberhard Goering[2] — [1]University of New South Wales and Australian Nuclear Science and Technology Organization, Sydney, Australia — [2]Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany — [3]University of Washington, Seattle, USA

Magnetic interface coupling effects such as exchange bias, the coupling of a ferromagnet to an adjacent antiferromagnet, are very difficult to probe directly by volume integrating techniques due to the small interface to volume ratio. During the last decade, soft x-ray resonant magnetic reflectometry has proven to be a powerful new tool to tackle this problem. Its combination of element selective magnetic sensitivity and high resolution depth profiling capability allows probing even very small magnetic effects at an interface. Investigations by different groups on a broad variety of exchange bias systems based on FeF2, MnPd, CoO, and IrMn have revealed a complex magnetic configuration at the interface. The antiferromagnet shows uncompensated rotatable magnetic moments which are confined to the direct neighborhood of the ferromagnet but also exotic pinned uncompensated magnetic moments. Especially the latter are interesting for our understanding of exchange bias since they should be responsible for the hysteresis loop shift in these systems. We review recent findings in the field and use them to illustrate the capabilities of SXRMR for the investigation of magnetic interface effects.

Topical Talk KR 7.2 Wed 10:00 BH 243

Orbital reflectometry of nickelate heterostructures — •Eva Benckiser — Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany

The occupation of *d*-orbitals has a key influence on the physical properties of transition metal oxides. Heterostructures of these oxides offer the possibility to control the orbital occupations because the electronic structure is very sensitive to changes in the transition-metal-oxygen bond distances induced by strain, dimensional constrains, and the chemical bonding to ions with different electronic configuration. However, atomic-scale modulations of the orbital occupation could thus far not be probed in a quantitative manner. We present results from a polarized soft x-ray resonant reflectivity study on superlattices composed of metallic $LaNiO_3$ and insulating $LaAlO_3$, $LaGaO_3$, or $DyScO_3$. We will demonstrate that it is possible to derive quantitative, spatially resolved orbital polarization profiles with differences of $\sim 3\%$ in the occupation of Ni e_g orbitals in adjacent atomic layers and discuss these results in context with recent theoretical predictions.[1–3] The possibility to quantitatively correlate theory and experiment on

the atomic scale opens up new perspectives for orbital physics in oxide heterostructures. [1] Chaloupka, J. and Khaliullin, G., Phys. Rev. Lett. 100, 016404 (2008). [2] Hansmann, P. et al., Phys. Rev. Lett. 103, 016401 (2009) and arXiv:1111.1111 [3] Han, M. J., Marianetti, C. A. & Millis, A. J. Phys. Rev. B **82**, 134408 (2010)

Invited Talk KR 7.3 Wed 10:30 BH 243

Manipulating magnetic and electronic ordering phenomena by electric fields and electromagnetic radiation — •Urs Staub — Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI. Switzlerand

Complex oxides may exhibit very interesting magnetic properties such as the appearance of the colossal magneto-resistance effect, complex charge and orbital ordering phenomena as well as cross-talk of magnetic and electric polarizations in multiferroics. These effects open up the possibility of manipulating magnetism by electric fields or electromagnetic radiation. Here I will give examples, which show how resonant soft x-ray magnetic diffraction can be used to monitor changes to the underlying magnetic structure. I will discuss how the insitu application of an electric field can change the magnetic order or domain population in a multiferroic, how spins can be canted by x-rays or how fast an antiferromagnetic phase transition can be induced by an ultrafast optical excitation, being monitored by ultrafast magnetic x-ray diffraction.

15 min. break

Topical Talk KR 7.4 Wed 11:15 BH 243

Theory of resonant x-ray spectroscopy — •M. W. Haverkort — Max-Planck Institute for Solid State Research, Stuttgart, Germany

Within the first half of this talk I will review the theoretical interpretation of x-ray absorption spectroscopy (XAS), elastic resonant x-ray diffraction (RXD) and resonant inelastic x-ray scattering (RIXS). I will briefly review how XAS can be used to measure the element specific magnetic susceptibility separated to its spin and orbital momentum contributions. Either with the use of sum-rules or by comparison to theory. Next, I will show how with the use of the optical theorem this understanding of XAS can be extended to RXD. This gives access to measure in a quantitative way the element resolved ordered spin and orbital moments. I will then continue to discuss RIXS, an inelastic scattering technique, which due to recent experimental improvements, allows one to measure dispersing magnetic excitations in small samples and thin films. Using the relations between inelastic scattering, elastic scattering and absorption spectroscopy a quantitative theory for RIXS is derived, which allows for an interpretation of the RIXS spectra very similar to Neutron spectroscopy.

In the last half of the talk several experimental results will be presented which show how these techniques can be used to gain understanding in the magnetic interactions in transition metal compounds.

Topical Talk KR 7.5 Wed 11:45 BH 243

Cycloidal Magnetic Order and Ferroelectricity: Manipulation and Imaging with Soft X-Rays — •Eugen Weschke[1], Enrico Schierle[1], Victor Soltwisch[1], Detlef Schmitz[1], Andrej Maljuk[1,2], and Dimitri Argyriou[1,3] — [1]Institut für komplexe magnetische Materialien, Helmholtz-Zentrum Berlin für Materialien und Energie, Germany — [2]Institut für Festkörperforschung, IFW Dresden, Germany — [3]European Spallation Source, Lund, Sweden

Materials with coupled order parameters, such as the magnetoelectric rare-earth manganites, offer interesting means of manipulation, like switching of magnetic order by electric fields. Ordering phenomena in these complex materials can be nicely studied by resonant scattering due to the element-selectivity of the method. In the soft x-ray region, in particular, spatial correlations involving the 3d and 4f electrons and their magnetic moments are directly addressed via dipole transitions. The method is applied to study cycloidal magnetic structures that occur in connection with ferroelectric order in $DyMnO_3$ and $GdMnO_3$, using circularly polarized synchrotron radiation to address the handedness of the structure [1]. The possibility to manipulate ferroelectric domains with the synchrotron beam is also demonstrated, which eventually provides a means to evidence ferroelectric polarization in cases where other methods are not conclusive or difficult to apply.

[1] E. Schierle et al., Phys. Rev. Lett. 105, 167207 (2010).

KR 7.6 Wed 12:15 BH 243

Local Magnetic Structure at the Fe_3O_4/ZnO Interface — •Sebastian Brück[1], Markus Paul[2], He Tian[3], Ozan Kirilmaz[2], Andreas Müller[2], Kai Fauth[1], Eberhard Goering[4], Jo Verbeeck[3], Gustaaf van Tendeloo[3], Michael Sing[2], and Ralph Claessen[2] — [1]University of New South Wales and ANSTO, Sydney, Australia — [2]Physikalisches Institut, Universität Würzburg, Würzburg, Germany — [3]Electron Microscopy for Materials Science, University of Antwerp, Antwerp, Belgium — [4]Max Planck Institute for Intelligent Systems (former Metals Research), Stuttgart, Germany

Magnetite, Fe_3O_4, is a half-metal with 100% spin polarization of the minority band at the Fermi level. This together with its good conductivity match to standard semiconductors makes it a promising candidate for polarized spin injection into semiconductor materials such as Si, GaAs, or ZnO. An important aspect for such applications is the magnetism directly at the interface between Fe_3O_4 and the semiconductor. Soft x-ray resonant magnetic reflectometry (XRMR) is a technique which is capable of providing structural and magnetic depth profiles with 0.1nm resolution. We present a detailed XRMR and electron energy loss spectroscopy (STEM/EELS) study of an epitaxial Fe_3O_4 thin film grown directly on a semiconducting ZnO substrate. Consistent chemical profiles at the interface between ZnO and Fe_3O_4 are found from XRMR and EELS. The magnetic depth profile of tetragonal Fe^{3+} and octahedral Fe^{2+} ions in Fe_3O_4 is derived with monolayer resolution and reveals a change in the Fe stoichiometry directly at the interface.

KR 8: Poster – 100 years since the Laue experiment: Topical aspects of diffraction and scattering (Joint Session KR, BP, DF, GP, MA, MI, MM; related SYXD)

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

KR 8.1 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.

KR 8.2 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 ($I^{\sim}|F|$) and imperfect crystals or ideal mosaic crystals due to the kinematical theory ($I^{\sim}|F|^*$). 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.

KR 8.3 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.

KR 8.4 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.

KR 9: Poster – Crystallography in Nanoscience

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

KR 9.1 Wed 15:00 Poster E

Phase-distribution in GaAs nanowires on Si (111) — •Andreas Biermanns[1], Steffen Breuer[2], Anton Davydok[1], Achim Trampert[2], Lutz Geelhaar[2], and Ullrich Pietsch[1] — [1]Universität Siegen, Festkörperphysik, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

The growth of semiconductor nanowires (NWs) has attracted significant interest in recent years due to their unique properties for possible novel semiconductor devices. However, many details of the growth mechanisms are not well understood. One particular problem during NW growth is the control of crystal structure, as NWs often adapt the cubic zinc-blende (ZB) or hexagonal wurtzite (WZ) structure. In addition, ZB rotational twins and stacking faults are often observed along the NW. As the structural composition usually varies between different NWs, individual characterization of a large ensemble of as-grown wires is often desired, but experimentally challenging. In this contribution we present a x-ray diffraction study of the distribution of ZB and WZ domains in GaAs nanowires grown on Si(111) across a large surface area. The GaAs NWs were grown by the Ga-assisted growth mode in molecular beam epitaxy. Using a nanometer-sized x-ray beam at the ESRF synchrotron source, the spatial distribution of particular sensitive Bragg-reflections was monitored, showing that the NWs grow predominantly in one ZB orientation without rotational twins. Close to the bottom of the NWs, WZ inclusions can be observed, whose position along the growth axis can be determined from the diffraction profile of the corresponding NW.

KR 9.2 Wed 15:00 Poster E

Analysis of defects in GaAs/InAs core/shell nanowires by means of Moiré pattern — •Torsten Rieger[1,2], Mihail Ion Lepsa[1,2], Thomas Schäpers[1,2], and Detlev Grützmacher[1,2] — [1]Peter Grünberg Institute - 9, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology

Semiconductor nanostructures containing heterostructures are promising for future (opto-) electronic devices. GaAs/InAs core/shell nanowires (NWs) are an example for such a self-assembled nanostructure having a high lattice mismatch. Apart from the usual mixture of the zinc blende and wurtzite crystal structure in III-V NWs, this lattice mismatch causes additional defects. Here, we present a detailed study about such defects observed in conventional bright field transmission electron microscopy (BF-TEM) and corresponding Moiré fringe pattern. Threading dislocations as well as different kinds of stacking faults are identified. The results are correlated with the growth mechanism of the InAs shell.

KR 10: Crystallography in Nanoscience

Time: Thursday 9:30–12:00 Location: E 124

Invited Talk KR 10.1 Thu 9:30 E 124

On polytypism in III-V nanowires — •Friedhelm Bechstedt[1], Abderrezak Belabbes[1], Christian Panse[1], Jürgen Furthmüller[1], Dominik Kriegner[2], and Julian Stangl[2] — [1]Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Johannes Kepler University, Altenbergerstrasse 69, 4040 Linz, Austria

Nanowires (NWs) based on III-V semiconductors, whose bulk crystals crystallize in zinc-blende structure, are usually grown in [111]B direction. Therefore, their bond stacking fluctuates, and the formation of different polytypes is a common phenomenon in NWs. The properties of the hexagonal 6H, 4H, and 2H polytypes are however modified with respect to the cubic zinc-blende (3C) structure.

A systematic study of structural and electronic properties of the Ga-V and In-V compounds (V = P, As, Sb) is reported for four polytypes. The lattice-constant and internal-cell parameters are derived within well-converged density-functional calculations within the local density approximation (LDA) and discussed versus the polytype hexagonality. The comparison with recent X-ray diffraction measurements shows excellent agreement and clear trends.

The quasiparticle electronic structures are computed with high accuracy including spin-orbit interaction applying a recent calculation scheme, the LDA-1/2 method. The fundamental gaps increase with the hexagonality. The results are used to derive band offsets between different polytypes. We predict a type-II heterocrystalline character for the junctions between two polytypes in agreement with spectroscopic studies.

KR 10.2 Thu 10:00 E 124

Crystal structure of InAs on Si(111) substrate — •Anton Davydok[1], Emmanouil Dimakis[2], Andreas Biermanns[1], Lutz Geelhaar[2], and Ullrich Pietsch[1] — [1]Festkörperphysik, Universität Siegen, Walter-Flex-Str. 3,57072, Siegen, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7,10117 Berlin, Germany

We present results of X-ray diffraction analysis of InAs nanowire (NW) grown by catalyze-free molecular beam epitaxy on silicon (111) substrate. Independent from lattice mismatch of 11% the NWs grow with

their bulk lattice parameter directly on bare silicon with absence of buffer layer or silicon native oxide layer. The structure of individual NWs has been characterized using a beam nano-focus beam spot of few 100nm*. Using coherent beam illumination certain Bragg peaks if individual NWs display speckle-like diffraction pattern due to particular sets of stacking faults separating wurzite and zinc-blende like structural units. Arrangement and density of stacking faults in particular NWs was estimated via modelling. In addition we characterized parasitic InAs islands appearing in addition to NWs which appear entirly in zinc-blende structure.

KR 10.3 Thu 10:20 E 124

In-situ 3D reciprocal space mapping during mechanical deformation — •Thomas Cornelius[1], Anton Davydok[2], Dina Carbone[3], Vincent Jacques[3], Raphael Grifone[3], Marie-Ingrid Richard[1], Till Hartmut Metzger[4], Tobias Schülli[3], Ullrich Pietsch[2], and Olivier Thomas[1] — [1]IM2NP, CNRS, Marseille, France — [2]Siegen University, Siegen, Germany — [3]ESRF, Grenoble, France — [4]MPI of Colloids and Interfaces, Potsdam, Germany

In recent years, low-dimensional materials attracted enormous attention due to size effects which originate from the spatial confinement of the nanostructures affecting their properties. At the beamline ID01 at ESRF, an in-situ AFM was developed for mechanical studies on nanostructures in combination with nanofocused XRD. The X-ray beam is focused to few hundred nanometers and the diffracted X-rays are recorded by a 2D detector. To record the complete structural change during deformation, it is mandatory to measure in-situ the 3D intensity distribution. Since any movement of diffractometer motors induces vibrations leading to the destruction of the AFM-tip and/or the nanoobject during compression, ordinary rocking curves cannot be applied. We developed a novel energy tuning approach which allows for the acquisition of 3D-XRD maps during in-situ compression tests and, thus, giving access to the deformation of the structure under investigation. Here, we will present in situ 3D-XRD studies on SiGe islands which served as a model system.

KR 10.4 Thu 10:40 E 124

Structure - stoichiometry relationship of mixed $Ce_{1-x}Pr_xO_{2-\delta}$ (x = 0-1) oxides on Si(111) — •Marvin Zoellner[1], Marcus Bäumer[2], Michael Reichling[3], Henrik Wilkens[3], Joachim Wollschläger[3], Peter Zaumseil[1], and Thomas Schroeder[1] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]Universität Bremen, IAPC, Leobener Str. NW2, 28359 Bremen — [3]Universität Osnabrück, Fachbereich Physik, Barbarastr. 7, 49076 Osnabrück, Germany

Cerium and praseodymium oxide thin films are of interest for model catalytic studies. When grown by molecular beam epitaxy on Si(111), CeO_2 exists in the fluorite lattice. Praseodymium prefers the 3+ state as Pr_2O_3, which has either a cubic bixbyite or hexagonal crystal structure. A mixture of both oxides enables to engineer the properties of the catalyst, due to different redox reactivities and lattice alteration. Before model catalytic studies can be carried out, the correlation between crystal structures and stoichiometries of the mixed $Ce_{1-x}Pr_xO_{2-\delta}$ layers must be clarified. We monitored the growth by reflection high energy electron diffraction. X-ray photoemission spectroscopy was applied to determine the stoichiometry. Laboratory and synchrotron based X-ray diffraction was carried out to investigate the crystal structure. The study revealed that $Ce_{1-x}Pr_xO_{2-\delta}$ keeps the Ce^{4+} related fluorite lattice for low praseodymium concentrations (x = 0.30). However, the crystal lattice is dominated by the Pr^{3+} state for medium (x = 0.65) and high (x = 0.75) Pr concentrations so that bixbyite and hexagonal structures are formed, respectively.

KR 10.5 Thu 11:00 E 124

Crystal size and axial stress effects on the B4 to B1 phase transition pressure in AlN and ZnO nanocrystals investigated with second harmonic generation (SHG) — •Leonore Wiehl, Lkhamsuren Bayarjargal, and Björn Winkler — Institut für Geowissenschaften, Goethe-Universität, 60438 Frankfurt/Main, Germany

The transition pressure from the hexagonal (B4) to the cubic (B1) phase is shifted to higher pressures in nanocrystals when compared to bulk crystals for GaN, InN, CdSe or ZnO [1]. Only in AlN a shift to lower pressure was reported [2]. The influence of deviatoric stress was shown to reduce the transition pressure of bulk ZnO from 11 to 9.3 GPa [3]. Here, we present our results on nanocrystals of ZnO and AlN. Pressures up to 30 GPa were generated in diamond anvil cells (DACs), loaded with Ne gas for hydrostatic or KCl for non-hydrostatic conditions. The phase transition was detected by the vanishing of the second harmonic generation signal when going from the acentric (B4) to the centrosymmetric (B1) phase. Our results confirm the shift of transition pressures in nanocrystalline ZnO by 2-3 GPa to higher and in AlN by ∼10 GPa to lower pressures relative to the bulk crystals in accordance with the values reported [1,2] in the hydrostatic case. For the non-hydrostatic loadings transition pressures were reduced by 2-3 GPa. Financial support from the DFG (Ba 4020) is gratefully acknowledged.

[1] J. Z. Jiang et al., Europhys. Lett. 50 (2000) 48-53 [2] Z. Wang et al., J. Phys. Chem. B 108 (2004) 11506-11508 [3] L. Bayarjargal et al., Appl. Phys. Lett. 95 (2009) 061907(3p)

KR 10.6 Thu 11:20 E 124

Manipulation of Ge quantum dot ordering in alumina matrix by deposition conditions — •Maja Buljan[1], Carsten Baehtz[2], Václav Holý[3], Nikola Radić[1], Olga Roshchupkina[2], Slawomir Prucnal[2], Arndt Muecklich[2], Václav Valeš[3], Sigrid Bernstorff[4], and Joerg Grenzer[2] — [1]Ruder Bošković Institute, Croatia — [2]Helmholtz Zentrum Dresden Rossendorf, Gremany — [3]Charles University in Prague, Czech Republic — [4]Sincrotrone Trieste, Italy

We present an investigation of ordering and PL properties of Ge QDs in an alumina matrix formed by magnetron-sputtering deposition of (Ge+Al2O3)/Al2O3 multilayers. The self-assembly process occurs during the deposition and results with the formation of three-dimensional quantum dots lattices. We investigate the dependencies of the size and ordering properties on the deposition temperature, rotation of the substrate holder and direction of the incoming flux of Ge during the deposition process. The results of the investigation show that tuning the deposition temperature enables manipulation with QD sizes and their mutual distances. We show that the ordering of QDs obtained by deposition on fixed substrate holder leads to the formation of a quantum dot crystal, while the rotation of substrate holder leads to randomly rotated domains with regular ordering. The observed phenomenon is explained by a combination of the surface morphology effect on the nucleation positions of Ge quantum dots with a lateral inhomogeneity of the ad-atom flux. In addition, we show that the resulting quantum-dot lattices have size-dependent PL properties.

KR 10.7 Thu 11:40 E 124

In-situ observation of the Self-assembled growth of ordered Ge nanocrystals embedded within a dielectrical matrix — •Joerg Grenzer[1], Maja Buljan[2], Olga Roshchupkina[1], Carsten Baehtz[1], and Václav Holý[3] — [1]Helmholtz Zentrum Dresden Rossendorf, Gremany — [2]Ruder Bošković Institute, Croatia — [3]Charles University in Prague, Czech Republic

We report on an in-situ X-ray investigation of a self-assembled growth of Ge nanocrystals embedded in a dielectrical matrix forming a *BCC*-like super structure. Such a material could be a key element for the development of a new generation of solar cells extending the spectral range for energy conversion. Using small angle scattering techniques and X-ray diffraction the formation of crystalline Ge nanoparticles during growth and annealing was studied in-situ at the BM20 beam line at that ESRF using a process chamber for magnetron sputter deposition and annealing that can be inserted into the goniometer. A single some 100nm thick $Ge+Al_2O_3$ layer using magnetron sputtering was deposited at an elevated substrate temperature. The self-assembly during growth or subsequent annealing results in the formation of a well ordered three-dimensional *BCC*-like quantum dot lattice within the whole deposited volume. The formed nanocrystals are very small in size ($< 4.0nm$), with a very narrow size distribution and a large spatial density. The parameters of the formed super structure can be directly influenced by changing the deposition parameters. The self-ordering of the quantum dots is explained by diffusion mediated nucleation and surface morphology effects.

KR 11: SYRS: Symposium Resistive Switching (joint symposium DS, DF, KR, HL – Organizers: Gemming, Dittmann)

Time: Thursday 15:00–17:30 Location: H 0105

Invited Talk KR 11.1 Thu 15:00 H 0105

Redox-based resistive memories - recent progress — •Rainer Waser — Forschungszentrum Jülich, 52425 Jülich, and IWE2, RWTH Aachen University, 52056 Aachen, Section Fundamentals of Future Information Technology (JARA-FIT), Germany

A potential leap beyond the limits of Flash (with respect to write speed, write energies) and DRAM (with respect to scalability, retention times) emerges from nanoionic redox-based switching effects encountered in metal oxides (ReRAM). A range of systems exist in which ionic transport and redox reactions on the nanoscale provide the essential mechanisms for memristive switching. In two classes, the so-called electrochemical metallization memories, ECM, and the so-called valence change memories, VCM, the electrochemical nature of these memristive effects triggers a bipolar memory operation. In yet another class, the thermochemical effects dominate over the electrochemical effects in metal oxides (so-called thermochemical memories, TCM) which leads to a unipolar switching as known from the phase-change memories. In all systems, the defect structure turned out to be crucial for the switching process. The presentation will cover recent progress in understanding the fundamental principles in terms of microscopic processes, switching kinetics and retention times, as well as device reliability of bipolar ReRAM variants. Despite exciting results obtained in recent years, several challenges have to be met before these physical effects can be turned into a reliable industrial technology.

Invited Talk KR 11.2 Thu 15:30 H 0105

Electric Formation of Metal/$SrTiO_3$ Junctions and its Correlation to Multi-Dimensional Defects — •Dirk C. Meyer[1], Hartmut Stöcker[1], Juliane Hanzig[1], Florian Hanzig[1], Matthias Zschornak[1,2], Barbara Abendroth[1], and Sibylle Gemming[2] — [1]TU Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Str. 23, 09596 Freiberg — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institut für Ionenstrahlphysik und Materialforschung, Bautzner Landstr. 400, 01328 Dresden

Regarding the successful use of strontium titanate with different doping within resistive switching memory cells, the presence of crystallographic defects seems to be an important prerequisite. Standard explanations for resistive switching rely on the redistribution of oxygen vacancies, however, this motion can be enhanced or prevented by higher-dimensional defects. Intrinsic defects in crystalline $SrTiO_3$ include point defects such as oxygen or strontium vacancies, line defects, stacking faults like Ruddlesden-Popper phases and precipitates (TiO_2, SrO etc.). Electric formation of the metal/oxide/metal cells is widely used as an initial step to enable resistive switching, but the interaction of the multi-dimensional defects during this treatment remains questionable. This talk will present several measurements that were performed in situ, i.e. during the application of an electric field, to investigate the effects of the electric formation on the real structure.

Invited Talk KR 11.3 Thu 16:00 H 0105

The Connecting between the Properties of Memristive Material Systems and Application Requirements — •Thomas Mikolajick[1,2], Stefan Slesazeck[1], and Hannes Mehne[1] — [1]NaMLab gGmbH, Nöthnitzer Str. 64, 01187 Dresden — [2]Chair of Nanoelectronic Materials Technische Universitaet Dresden

In the last years large progress has been made to identify switching mechanisms in resistive switching materials and connect these to the materials systems used. The different switching mechanisms result in significantly different I-V characteristics of the switching behavior. As an example the switching can be bipolar or unipolar, abrupt or continuous etc. Additionally parameters like switching power, retention and endurance may show a characteristic fingerprint. In this talk the main mechanisms like thermo-chemical switching, valence change switching or electrochemical switching are compared to the requirements for different types of semiconductor memories like nonvolatile RAM, high density data memories or embedded memories and an assessment of the prospects of the different mechanisms for each system is given. Non-memory applications of memristive switching like xeromorphic circuits will also be taken into consideration.

Invited Talk KR 11.4 Thu 16:30 H 0105

Mechanism of resistive switching in bipolar transition metal oxides — •Marcelo Rozenberg — CNRS - LPS, Universite de Paris-Sud, 91405 Orsay, France

Resistive random access memories (RRAM) composed of a transtition metal oxide dielectric in a capacitor-like structure is a candidate technology for next generation non-volatile memory devices. We introduce a model that accounts for the bipolar resistive switching phenomenom observed in many perovskite transition metal oxides. The numerical study of the model predicts that strong electric fields develop in the highly resistive dielectric-electrode interfaces, leading to a spatially inhomogeneous distribution of oxygen vacancies and a concomitant nonvolatile resistance memory effect. The theoretical results of the model are validated by successful comparison with non-trivial resistance hysteresis loops measured in cuprate YBCO and manganite PCLMO samples. Insights from the model simulations are used to propose a novel multi-level and non-volatile memory cell. We shall present results for an implementation of a 6-bit multi-leve memory cell device.

Invited Talk KR 11.5 Thu 17:00 H 0105

Resistive switching memories: Mechanisms, modeling and scaling — •Daniele Ielmini — Dipartimento di Elettronica e Informazione and IUNET, Politecnico di Milano, Piazza L. da Vinci 32, 20133 Milano, Italy

Resistive switching memory (RRAM) devices are proposed as next mainstream technology for nonvolatile memories below the 10-nm node. However, to speed up the industrial development of RRAM, the research must still address several open issues, such as identifying a suitable select device, understanding the switching mechanism and predicting the device scalability.

In this talk, I will show experimental results for bipolar RRAM devices based on metal oxides (mostly HfO_x), evidencing that the switching mechanism is a temperature and field-activated ion migration. Based on these experimental evidences, I will provide an analytical model for resistive switching which can be applied to oxide-based RRAM and chalcogenide-based conductive bridge RAM (CBRAM). The model allows for space, time and energy extrapolation for future RRAM generations. The extension of the analytical approach to a self-consistent numerical model for ion migration will be shown. The scaling tradeoff with reliability, e.g. random telegraph noise and data retention, will be finally discussed.

KR 12: Mitgliederversammlung FG Kristallographie

Time: Thursday 17:45–18:30 Location: E 124

Mitgliederversammlung FG Kristallographie