Crystallography Division
Fachverband Kristallographie (KR)

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Overview of Invited Talks and Sessions

(lecture rooms H3, H4, and H9; Poster A)

Invited Talks

KR 2.1	Tue	9:30–10:15	H9	**Coherent X-ray Diffraction for mapping strains in ZnO Nanocrystals** — •Ian Robinson

Sessions

KR 1.1–1.3	Sun	16:00–18:15	H4	**Tutorial: Functional (oxide) single crystals and epitaxial films - from growth to function**
KR 2.1–2.11	Tue	9:30–13:00	H9	**Crystallography in nanoscience**
KR 3.1–3.5	Wed	15:00–17:30	Poster A	**Poster: Crystallography in Nanoscience**
KR 4	Thu	17:00–18:00	H12	**Mitgliederversammlung KR**
KR 5.1–5.4	Wed	10:15–11:30	H4	**Topical Session Photovoltaic Materials I (with MM and BV MatWerk)**
KR 6.1–6.6	Wed	11:45–13:15	H4	**Topical Session Photovoltaic Materials II (with MM and BV MatWerk)**
KR 7.1–7.4	Wed	14:45–15:45	H4	**Topical Session Photovoltaic Materials III (with MM and BV MatWerk)**
KR 8.1–8.9	Mon	10:15–12:45	H3	**Multiferroics I (Joint Session of MA, DF, KR, DS)**
KR 9.1–9.14	Mon	14:00–17:45	H3	**Multiferroics II (Joint Session of MA, DF, KR, DS)**
KR 10.1–10.80	Tue	10:45–13:45	Poster A	**Poster: Multiferroics (with MA, DF, KR, DS)**

Annual General Meeting of the Crystallography Division

Donnerstag 17:00–18:00 Raum H12

- Bericht der Fachverbandsleiterin
- Zukünftige Weiterentwicklung des Fachverbands Kristallographie
- DPG-Tagung 2011
- Aktivitäten zum Laue-Jahr 2012
- Verschiedenes

KR 1: Tutorial: Functional (oxide) single crystals and epitaxial films - from growth to function

Time: Sunday 16:00–18:15 Location: H4

Tutorial KR 1.1 Sun 16:00 H4

Influence of ferroelectric phase transitions on the melt growth of bulk oxide crystals — •Manfred Mühlberg and Manfred Burianek — Universität zu Köln, Institut für Kristallographie, Zülpicher Str. 49 b, 50674 Köln

Various applications in electronics, linear and nonlinear optics and other fields are connected with components taken from bulk single crystals. Also the determination of several fundamental physical properties like dielectric constants, piezo- or pyroelectric tensor components requires single crystalline samples. To meet these requirements one is primarily concerned with obtaining crystals of predetermined size with a high degree of structural perfection and a well-determined chemical composition.

In this introductory lecture, the most important growth methods from the melt and from high temperature solutions will be presented focusing on examples of selected ferroelectric perovskites and tetragonal tungsten bronzes. The chemical and thermophysical properties of the multi-component materials also represented by phase diagrams determine the synthesis steps and the details of the growth process.

A short overview of the defect types depending on the material properties and growth parameters will be given. Some options for reducing the defect content and improving the crystalline quality are reported for potassium lithium niobate and calcium barium niobate. Finally, a special attention is focused on the types and the influence of ferroelectric phase transitions being occuring between the growth temperature and the crystalline state at room temperature.

Tutorial KR 1.2 Sun 16:45 H4

Electromechanical properties of crystals — •Eiken Haussühl — Institut für Geowissenschaften / Abt. Kristallographie, Goethe Universität Frankfurt

The knowledge of physical properties of crystals as bulk materials is rather limited in comparison to the huge number of known crystal structures. In this introductory tutorial fundamental aspects of crystal physics will be presented. The lecture is intended to provide the basics for the understanding of the distinctiveness of crystalline compounds and to bring closer the phenomenological aspects under the influence of symmetry. It is also intended to highlight practical considerations for the measurement of selected tensorial properties. The main part will be focused on the mechanical properties of the bulk material like thermal expansion, elasticity and on electrical properties like piezoelectricity. Different effects arising from phase transition of selected organic and inorganic materials like oxides will be discussed.

Tutorial KR 1.3 Sun 17:30 H4

Epitaxial ferroelectric oxide thin films, nanostructures, and superlattices — •Dietrich Hesse, Ionela Vrejoiu, and Marin Alexe — Max Planck Institute of Microstructure Physics, Halle, Germany

Epitaxial ferroelectric thin films, nanostructures and superlattices represent a particularly interesting part of functional materials. In this tutorial, fundamental terms of epitaxial growth will be presented, along with a detailed characterization of growth-structure-property relations of a number of examples of perovskite-type ferroelectric structures. E.g., it will be shown how remanent polarization and switchability of pulsed-laser deposited $Pb(Zr,Ti)O_3$ (PZT) epitaxial thin films depend on the defect content (threading dislocations, stacking faults), and how the properties of antiferroelectric/ferroelectric $PbZrO_3$/PZT superlattices depend on the thickness of the individual layers via strain. The properties of epitaxial, ferroelectric $(Bi,La)_4Ti_3O_{12}$ nanostructures and Pt/PZT/Pt nanocapacitors of sub-100 nm size are shown to be determined by crystallographic orientation, crystal perfection, and size. The role of 2D defects will be highlighted, viz. ferroelectric 90 degree domain boundaries in epitaxial PZT films serving as nucleation centers for 180 degree switching, and the atomic structure of 180 degree boundaries influencing the switching process. Overall the interesting physical properties of epitaxial functional perovskite structures are discussed in terms of growth, crystal orientation, defect type, defect content, and strain.

KR 2: Crystallography in nanoscience

Time: Tuesday 9:30–13:00 Location: H9

Invited Talk KR 2.1 Tue 9:30 H9

Coherent X-ray Diffraction for mapping strains in ZnO Nanocrystals — •Ian Robinson — London Centre for Nanotechnology — Diamond Light Source

In condensed matter physics, we consider nanometre-sized crystals to be a new frontier of opportunity to tailor physical properties using "size" as a control variable. However, when we think about nanostructures, we must reconsider the standard bulk concepts of lattices and crystal defects. Changes here provide nanomaterials with new and exciting properties. This talk will illustrate how coherent X-ray diffraction at a 3rd generation synchrotron source can be used to obtain quantitative three-dimensional maps of the deformation of a crystal from its equilibrium lattice spacing. To invert the diffraction, we have solved the crystallographic "phase problem" by oversampling using a support-constrained HIO algorithm. The ZnO crystals we have been investigating were attached by bonding to a SiO_2 substrate and show internal strain arising from accidental damage during manipulation. Use of more than one Bragg peak from the same crystal has allowed components of the full strain tensor to be mapped inside the crystal.

"Coherent Diffraction Imaging of Strains on the Nanoscale", Ian Robinson and Ross Harder, Nature Materials 8 291-298 (2009)

"Three-dimensional imaging of strain in a single ZnO nanorod", M. C. Newton, S. J. Leake, R. Harder and I. K. Robinson, Nature Materials (2010)

KR 2.2 Tue 10:15 H9

X-ray characterisation of single GaAs nanorods grown on Si — •Andreas Biermanns[1], Anton Davydok[1], Steffen Breuer[2], Lutz Geelhaar[2], and Ullrich Pietsch[1] — [1]Universität Siegen, Festkörperphysik, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Semiconductor nanorods are of particular interest for new semiconductor devices. The nanorod approach can be used to form radial or axial heterostructures of materials with a large lattice mismatch. For the inspection of average structural parameters of the nanorods, typically x-ray or electron diffraction techniques are used. Alternatively, transmission electron microscopy can be used to inspect few individual nanorods after respective sample preparation. Complementary, recent developments in x-ray optics allow to focus a synchrotron beam down to the nanometer scale and to perform nondestructive diffraction studies at several individual nano-objects grown the same substrate. In this contribution we report on x-ray diffraction studies at individual GaAs nanorods grown Au seed-free on a Si[111] substrate. Due to the nanometer-sized x-ray beam, size and lattice parameters of individual nanorods could be measured and compared to the value obtained from the whole ensemble. Using the coherence properties of the focused beam we could observe speckle-like interference fringes in the surrounding of particular sensitive Bragg reflections which are a measure for the appearance of stacking faults within the nanorods. The separation of the speckles could be used to estimate the number of stacking faults and the size of the coherently scattering nanorod-segments.

KR 2.3 Tue 10:30 H9

Mechanical properties of single nanostructures investigated by in-situ AFM and micro-XRD — •Thomas Cornelius, Thomas Scheler, Rogerio Magalhães-Paniago, and Till Hartmut Metzger — ESRF, 38043 Grenoble Cedex, France

In recent years, nanostructures attracted enormous attention due to size-effects influencing the structural, optical, electrical, and mechanical properties of materials with low dimensions. Concerning the me-

chanical properties mainly the plastic regime was explored showing a trend that "smaller is stronger". In contrast, studies of the elastic behaviour of nanowires revealed contradictory results concerning the influence of size-effects on the elasticity. To investigate single nanoobjects in the elastic regime, we combined an in-situ AFM with XRD in a microfocused beam. The AFM is used to image the sample surface, to select an individual nanostructure, and to apply pressure on a chosen object. Due to the interaction between the AFM-tip and the compressed object the resonance frequency of the AFM force sensor shifts to larger values enabling us to derive the stiffness of the contact area. Simultaneous to the pressure application, XRD images around a pre-defined Bragg peak are recorded. These images allow for the determination of the elastic lattice parameter change in-situ. From the contact stiffness and the lattice parameter change, the Young modulus of an individual nanoobject is derived. Here, we will present results both for SiGe islands grown by liquid-phase epitaxy on Si wafers and GaAs nanorods created by selective-area metal organic vapor phase epitaxy on GaAs substrates.

KR 2.4 Tue 10:45 H9

Correlation of structure and conductance in nanowires and nanotubes — •Sibylle Gemming — Institute of Ion Beam Physics and Materials Research, FZ Dresden-Rossendorf, P.O. Box 51 01 19, D-01314 Dresden, Germany.

In nanostructured materials spatial confinement effects lead to structure-dependent deviations from the bulk transport properties. Such modifications may in part be accounted for by classical transport simulations, but a microscopically more detailed and mostly parameter-free picture is obtained from quantum-mechanical density-functional theory (DFT). DFT calculations yield the atom arrangement and electronic structure of nanotubes and nanowires in the electronic ground state. Additionally, an extension by a Green's function formalism leads to the determination and analysis of electronic transport through contacted nanostructures. A combination of both approaches allows to correlate structural and transport properties of nanostructures. The applicability of this approach will be demonstrated for a mechanically triggered metal-insulator transition in nanowires.

[1] Kibsgaard et al. *Nano Lett* **8** (2008) 3928; [2] Popov et al. *Nano Lett* **8** (2008) 4093.

KR 2.5 Tue 11:00 H9

The X-ray investigation of GaAs nanorods grown onto Si[111] substrate — •Antron Davydok[1], Andreas Biermanns[1], Ullrich Pietsch[1], Steffen Breuer[2], and Lutz Geelhaar[2] — [1]University of Siegen, Siege, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Nanorods (NR) are of particular interest due to the ability to synthesize single-crystalline 1D epitaxial structures and heterostructures in the nanometer range. It was found that nearly any AIIIBV semiconductor material can be grown as NRs onto another AIIIBV or group IV [111] substrate independent from lattice mismatch. We presented an X-ray characterization of GaAs NRs on Si [111] grown by gold-seed assist MBE method. We concentrated our research on 4 samples with different growth time: a) at 5s growth time several island but no NWs are found on the surface; b) at 60s first NWs appeared; c) at 150s the size of rods is increased; d) at 1800s many NWs occupy the whole surface. Using synchrotron radiation we have performed experiments in symmetrical and asymmetrical out-of plane scattering geometry and depth resolved grazing-incidence diffraction. Combining the results we were able to determine the strain gradient between wurzite like NR and zincblende substrate. Using particularly asymmetric wurzite-like reflections under coherent beam illumination we could quantify the number of stacking faults In the talk we present details of the analysis and first simulation results.

15 min. break

KR 2.6 Tue 11:30 H9

Inspection of single CdSe nanowires by use of microfocused x-ray diffraction — •Özgül Kurtuluş[1], Zhen Li[2], Bahia Arezki[3], Andreas Biermanns[3], and Ullrich Pietsch[3] — [1]Doguş University, Istanbul,Turkey — [2]University of Queensland, Brisbane, Australia — [3]University of Siegen, Siegen, Germany

The morphology of CdSe nanowires (NW) can easily be controlled by various growth methods. In this study, CdSe NWs are prepared by solution-liquid-solid (SLS) approach providing needle-shaped wires of about 60nm in diameter and several microns in length. To make x-ray single NW inspection possible, the NWs were dispersed in toluen and hexadecylamine, homogenized by centrifugation and finally spin-coated on silicon substrate. SEM images revealed that the NWs are randomly oriented with length axis parallel to the substrate. However, at selected areas, the distance between neighboured NWs is in the order of one micron. These samples were investigated by x-ray diffraction using a 300nm x 600nm micro-focus at beamline ID1 of ESRF. Diffraction from 110W/2-20ZB basal plane was selected for single nanowire inspection. In order to measure various single objects subsequently, the sample was laterally scanned through the beam keeping the diffraction angle fixed. It was observed that the individual NWs differ slightly in peak position and peak width. From powder diffraction, it is known that NWs consist of an admixture of a wurtzite (W) and zinc-blende (ZB) structure units and the coherent illumination of sample by the micro-focus enables to visualize these zinc-blende and wurzite units seperated by stacking faults.

KR 2.7 Tue 11:45 H9

Nanolaminate's thermal conductivity at low temperatures — •Erik Mehner[1], Stefan Braun[2], Mathias Dörr[3], and Dirk C. Meyer[1] — [1]Institut für Strukturphysik, Technische Universität Dresden,D-01062 Dresden,Germany — [2]Fraunhofer IWS, Abteilung Röntgen-EUV-Optik Dresden — [3]Insitut für Festkörperphysik, Technische Universität Dresden,D-01062 Dresden,Germany

Due to their importance for application in solar cells and gas turbines thermal barrier coatings were investigated.

Current understanding of the heat conductivity between nanoscale interfaces is still incomplete and subject of ongoing scientific work. The 3-omega-method is a well established method for thin-film thermal conductivity measurements. [1]

First results of the implementation of a low temperature 3-omega-measurement which was devised to seperate phononic and electronic heat conduction with respect to the conception of an thermal barrier coating are presented. Likewise the morphological and structural aspects of the multilayer coatings, were included in design considerations. After the setup's qualification with glass-substrates W/Al2O3-multilayer samples were examined. Their thermal conductivity of 0,6 Watts per meter Kelvin at room temperature is confirmed. [2] Alternatively the system ZrO2/Al2O3 was investigated showing good suitability for thermal barrier coating up to at least temperature of 800°C.

[1] R. M. Costescu, David G. Cahill, F. H. Fabreguette, Z. A. Sechrist, and S. M. George. Science, 303(5660), 989-990, (2004)

[2] David G. Cahill. Rev. Sci. Instrum., 61(2), 802-808, (1989)

KR 2.8 Tue 12:00 H9

Polarization dependent Diffraction Anomalous Fine Structure of rutile TiO_2 001 and 111 reflections — •Matthias Zschornak[1,2], Carsten Richter[1], Hartmut Stöcker[1], Tilmann Leisegang[1], Sibylle Gemming[2], and Dirk C. Meyer[1,3] — [1]Nachwuchsgruppe Nanostrukturphysik, Institute of Structural Physics, TU Dresden, Germany — [2]Institute of Ion Beam Physics and Materials Research, FZ Dresden-Rossendorf, Germany — [3]Institute of Experimental Physics, TU Bergakademie Freiberg, Germany

Energy and polarization dependent *Diffraction Anomalous Fine Structure* (DAFS) also known as *Anisotropic Anomalous Scattering* (AAS) can be employed in addition to *X-ray Absorption Fine Structure* (XAFS) to study electronic transitions from core states to unoccupied states. Here, we present results from resonant X-ray diffraction experiments on TiO_2 rutile, space group (136) $P4_2/mnm$. For this model structure, site symmetry information was extracted from determination of the structure factor tensor by refining elements of Ti atomic scattering factor tensors. Influences of oxygen vacancies on the anomalous scattering contributions have been studied on a series of rutile wafers of different oxygen concentration. Samples investigated were $10 \times 10 \times 1$ mm^3 single crystal wafers and experiments were carried out at DESY/HASYLAB beamlines C and E2 using a Si (111) double crystal monochromator in the vicinity of the Ti-K absorption edge. Considered reflections include the 'forbidden' 001 and allowed 111 reflection.

KR 2.9 Tue 12:15 H9

Electric Field Induced Structural Modifications in Metal/$SrTiO_3$ Junctions and their Resistive Properties —

•Hartmut Stöcker[1,2], Juliane Seibt[2], Florian Hanzig[2], Susi Wintz[2], Matthias Zschornak[1], and Dirk C. Meyer[2] — [1]TU Dresden, Institut für Strukturphysik, Zellescher Weg 16, 01062 Dresden — [2]TU Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Straße 23, 09599 Freiberg

In oxides with perovskite-type of structure, mobile oxygen can cause the formation of non-stoichiometric regions when an electric field of sufficient strength (∼1000 V/mm) is applied. Our *in-situ* investigations of metal/$SrTiO_3$ junctions revealed reversible structural changes at room temperature caused by a systematic field-induced redistribution of oxygen. The investigations were carried out using wide-angle X-ray scattering, X-ray absorption spectroscopy, photoluminescence, nanoindentation and time-dependent electric *I-U* measurements.

Motivated by the successful use of $SrTiO_3$ with different doping metals for memory cells on the basis of resistive switching combined with the findings on the major importance of oxygen vacancy redistribution, we want to show the possibility of realizing a resistance change memory based on vacancy-doped $SrTiO_3$. The formation of corresponding metal/$SrTiO_3$ junctions in an electric field will be discussed as well as the switching between ohmic and Schottky-type resistive properties. A notable hysteresis in the *I-U* characteristics can be used to carry out Write, Read and Erase operations to test the memory cell properties of such junctions.

KR 2.10 Tue 12:30 H9

Microstructure study of gold-zirconia yolk-shell nanostructures using XRD line profile analysis — •Arti Dangwal Pandey[1], Robert Güttel[1], Matteo Leoni[2], Ferdi Schüth[1], and Claudia Weidenthaler[1] — [1]Max-Planck-Institut für Kohlenforschung, Mülheim (Ruhr), Germany — [2]University of Trento, Italy

The detailed microstructure study of gold nanoparticles encapsulated inside crystalline zirconia hollow-spheres is presented. This system is a potential nano-catalyst for CO-oxidation such as in automotive exhaust gas treatment.[1] The crystalline zirconia shell of 200 nm diameter separates the 15 nm gold nanoparticles from each other and provides high temperature stability to this system. To retrieve the microstructure details like size distribution, dislocation density, dislocation character, and defect content from the powder diffraction data of this two phase nanostructure system, we used whole powder pattern modeling (WPPM) for line profile analysis [2]. A series of diffraction and microscopic measurements were performed to investigate how the microstructure of these nanostructures evolves after some chemical and heat treatments. The observed variation in the crystallite size and defect contents after gold-leaching or quenching of the as prepared material from 900°C will be discussed in detail and the influence on the catalytic activity of gold nanoparticles will be presented.

1. P.M. Arnal, M. Comotti and F. Schüth, Angew. Chem. Int. Ed., 2006, 45, 8224.

2. Scardi P. and Leoni M., Acta Cryst. A, 2002, 58, 190-200.

KR 2.11 Tue 12:45 H9

Confocal Raman investigation of the zoning in synthetic $Ca(CO_3,CrO_4)$ crystals — •Alexander M. Gigler[1,2], Nuria Sanchez-Pastor[1], Guntram Jordan[1], and Wolfgang W. Schmahl[1,2] — [1]Section Crystallography, LMU-München, D-80333 München — [2]CeNS, LMU-München, D-80799 München

Due to its high mobility and toxic effects even in very low concentrations, hexavalent chromium (Cr^{6+}) is known as one of the most common environmental contaminants resulting from its widespread use in industrial applications.[1] Here, we present data on the crystallization of $CaCO_3$ in a silica hydrogel medium in the presence of different concentrations of Cr^{6+}.[2,3] Morphological changes in calcite correlate with chromium incorporation in its structure. This incorporation is evidenced by the appearance of new vibrational bands in the Raman spectrum, which are consistent with the substitution of carbonate groups by chromate groups. Therefore, chromium incorporation into calcite could be described as an anionic solid solution with a very limited maximum chromate concentration. By means of Raman microscopy, we observed a zoning of the crystals. The central region was chromium-rich, while pure calcite was present in the outer region due to a depletion of chromium in the gel. Incorporation of chromium into calcite may solve a major environmental problem, since toxic chromium can be rendered harmless.

[1] Katz, Salem: The Biological and Environmental Chemistry of Chromium, VCH, 1994. [2] Henisch: Crystal growth in gels, Dover Publ., 1996. [3] Cruz et al. Geochim. Cosmochim. Acta 73, A252, 2009.

KR 3: Poster: Crystallography in Nanoscience

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

KR 3.1 Wed 15:00 Poster A

Physical aspects of the growth dynamics of plasmonic structures — •Merle Becker[1], Bernhard Grotz[1], Jens Pflaum[2], Fedor Jelezko[1], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany — [2]Inst. Exp. Phys. VI, Julius-Maximilians Univ. and ZAE Bayern, 97074 Wuerzburg, Germany

In recent years, the importance of nanostructured materials for applications in e.g. nano-optics, plasmonics and as components of sensing devices strongly increased. Production by lithographic methods like optical, e-beam or ion-beam lithography [1] results in controllable and reproducible structures, however with the drawback of being highly intricate and expensive. In this contribution we demonstrate an alternative approach to compass these problems which is the use of chemical syntheses in combination with self-aggregation [2]. Silver nanowires grown in solution are investigated to optimize their performance as plasmon waveguides and antennae. Distributions of length and diameter in dependence on time and consequential development of aspect ratios of nanowires reveal influences of PVP on surface energies of participating faces. Broadenings of the distributions of length and diameter during growth are investigated and can be related to surface roughening of the (111) and (100) faces during growth process.

[1] Pelton, M. Laser&Photon. Rev. 2, 136-159 (2008) [2] Xia, Y. et al. Adv. Mater. 15, 353-389 (2003)

KR 3.2 Wed 15:00 Poster A

Structure of W-C-nanodots prepared by focused electron beam induced deposition as determined by electron diffraction — •Iryna Andrusenko[1], Tatiana Gorelik[1], Andrew Stewart[1], Ute Kolb[1], Mike Strauss[2], Roland Sachser[3], Fabrizio Porrati[3], and Michael Huth[3] — [1]Institute of Physical Chemistry, University Mainz, Mainz, Germany — [2]Department of Structural Biology, MPI of Biophysics, Frankfurt/Main, Germany — [3]Physikalisches Institut, Goethe University, Frankfurt/Main, Germany

Ordered two-dimensional nanodot lattices of various lattice pitches were fabricated from $W(CO)_6$ precursor by focused electron-beam-induced deposition (FEBID) on amorphous carbon or silicon templates. Electron transmission microscopy images and diffraction patterns were collected at 300 kV with a FEG-TEM. Tomographic reconstructions from images taken at liquid nitrogen temperature were generated by weighted back-projection from 85 zero-loss filtered images taken over a tilt range of ±63 degrees at a nominal defocus of -1 μm and a magnification of 48000. Electron diffraction patterns, providing resolution superior to imaging techniques, were performed using selected area electron diffraction as well as a semi-parallel beam of 50 nm diameter. Diffraction patterns of the full 1x1 μm dot lattice area delivered a mean distance of about 2.3 Å indicating a W-C bond length. Diffraction patterns of single particles have been collected in order to reconstruct high resolution images. The structural features of FEBID grown W-C-nanodots investigated by electron diffraction were subsequently correlated with Raman spectroscopy results.

KR 3.3 Wed 15:00 Poster A

Detailed Analysis of the Small Angle X-Ray Scattering of ordered mesoporous titania compounds calcined at different temperatures — •Lars Robben[1] and Adel A. Ismail[2] — [1]Institut für Mineralogie und ZfM, Leibniz Universität Hannover — [2]Institut für Technische Chemie und ZfM, Leibniz Universität Hannover

Small Angle X-Ray Scattering (SAXS) is a powerfull method for the characterization of ordered mesoporous materials (OMMs). OMMs are principially two-phases systems: A material, for example SiO_2 or

TiO_2, contains pores with a diameter between 2-50 nm with a regular ordering. The ordering scheme as well as the size and shape of the pores can be controlled by the synthesis conditions. In SAXS experiments the electron density difference between the pores and the material generates Bragg-Reflections which can be used to elucidate the type of crystallographic lattice of the ordering scheme of the pores and to calculate the lattice parameter. An important point with respect to the technical application of TiO_2-OMMs is the crystallinity of the material because a higher crystallinity ensures a better photoactivity for catalytic purposes. Here we present SAXS investigations of TiO_2-OMM calcined at different temperatures and review the assignment of the symmetry group. Furthermore we clarify the main processes which determine the development of the OMM during calcination. Most important in this respect is the interdependency between the crystallinity of the material and the quality (that is the pore shape and the regularity of the lattice) of the mesoporous system.

KR 3.4 Wed 15:00 Poster A

Generation of hard X-ray radiation using the triboelectric effect — •Maximilian Rühl[1], Emanuel Gutmann[1], Erik Mehner[1], Hartmut Stöcker[1], and Dirk C. Meyer[2] — [1]Nachwuchsgruppe Nanostrukturphysik, Institut für Strukturphysik, TU Dresden, 01069 Dresden — [2]Institut für Experimentelle Physik, TU Bergakademie Freiberg, 09596 Freiberg

To meet the demands of upcoming imaging for medical demands and scientific methods for structure investigation, generation of X-rays using miniaturized radiation sources is an interesting field of research. Beside approaches based on the ionizing and electron accellerating properties of high electric fields around pyroelectric crystals also the use of a tribomicroplasma generated in the vicinity of the peeling point of two different polymers is promising [1]. We report on the generation of hard X-ray radiation by crawling various peeling tapes in a medium vacuum. Beside vacuum housing and pumps as instrumentation only an electric motor, two rolls and a metal foil as target material are necessary. The spectral distribution of thus generated X-rays was analyzed using an energy dispersive Si (Li) detector. In dependence of peeling speed, pressure and choice of polymer material electrons with energies high enough to excite characteristic X-ray emission in the hard X-ray region are produced. The results are discussed in terms of theory of triboelectricity [2]. [1] C. G. Camara et al. Correlation between nanosecond X-ray flashes and stick-slip friction in peeling tape, Nature 455 (2008) 1089-1092 [2] P. A. Thießen, K. Meyer, G. Heinicke, Grundlagen der Tribochemie (1967) Akademie-Verlag, Berlin

KR 3.5 Wed 15:00 Poster A

Oxygen vacancy contribution on Anisotropic Anomalous Scattering of rutile TiO_2 — •Carsten Richter[1], Matthias Zschornak[1], Hartmut Stöcker[1], Tilmann Leisegang[1], Dmitri Novikov[2], and Dirk C. Meyer[3] — [1]Nachwuchsgruppe Nanostrukturphysik, Institute of Structural Physics, TU Dresden, Germany — [2]Hamburger Synchrotronstrahlungslabor HASYLAB at DESY, 22603 Hamburg, Germany — [3]Institute of Experimental Physics, TU Bergakademie Freiberg, Germany

The unique potential of *Anisotropic Anomalous Scattering* (AAS) for investigation of randomly distributed point defects has been discussed theoretically by Dmitrienko and Ovchinnikova [1]. Here, we use this approach to study influences of oxygen vacancies in rutile TiO_2 on the resonant scattering contributions at the Ti-K absorption edge. First energy dependent AAS experiments have been performed on a series of single crystal wafers with different oxygen concentrations obtained by annealing at a temperature of 800 °C in a vacuum of about 10^{-6} mbar for different durations. Measurements were carried out at DESY/HASYLAB on 'forbidden' 001 and allowed 111 reflections. An interpretation based on vacancy-induced static Ti displacements from high- to low-symmetry positions will be presented.

[1]*V.E. Dmitrienko, E.N.Ovchinnikova: Acta Cryst. A56 (2000) 340-347.

KR 4: Mitgliederversammlung KR

Time: Thursday 17:00–18:00 Location: H12

Mitgliederversammlung FV Kristallographie

KR 5: Topical Session Photovoltaic Materials I (with MM and BV MatWerk)

Time: Wednesday 10:15–11:30 Location: H4

Topical Talk KR 5.1 Wed 10:15 H4

Solar cell absorbers made from rust ? - Stacked-Elemental-Layer-RTP and corrosion of alloys — •Rainer Hock, Roland Schurr, and Astrid Hölzing — University Erlangen-Nürnberg, Chair for Crystallography and Structural Physics, Staudtstraße 3, D-91058 Erlangen, Germany

Semiconducting absorber materials for thin film photovoltaics like $Cu(In,Ga)(S,Se)_2$ can be crystallised by heating thin metallic films in chalcogenide atmospheres. This process is known under the acronym SEL-RTP (Stacked Elemental Layer - Rapid Thermal Processing). In the initial stages of this process, the metallic films are attacked by sulfur, selenium or both, forming often a variety of metal chalcogenides. We had a 'second look' on the initial stage of SEL-RTP for the fabrication of absorber materials for thin film photovoltaic applications. This first step is the corrosion of the metal alloys in chalcogenide atmospheres. The different view on the fabrication process may allow to learn from a field of scientific research which was driven mainly by the oil and chemical industries in the second half of last century. At that time, the focus was directed on the search for corrosion resistant metal alloys for use in sulfur containing atmospheres or liquids. Through a reversed view, SEL-RTP may be seen as the desired and complete corrosion of thin metallic films. At the end of the corrosion process a polycrystalline thin film, monophase and with the desired material properties is hopefully produced. Controlled corrosion than leads to a functional, e.g. photovoltaically active thin film.

KR 5.2 Wed 10:45 H4

Amorphous / crystalline silicon heterojunctions: Changes of structural and electronic properties upon low-temperature annealing — •Hannes Ner Beushausen, Tim Ferdinand Schulze, and Lars Korte — Silicon Photovoltaics, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Solar cells based on amorphous/crystalline silicon (a-Si:H/c-Si) heterojunctions have gained much attention due to their high conversion efficiency. In order to increase the open circuit voltage V_{oc} of these solar cells, the prime objective is to 'passivate' the a-Si:H/c-Si interface, i.e. to suppress interface recombination of photogenerated charge carriers by saturating recombination-active dangling bonds.

Commonly, thin (3-10nm) undoped, nominally intrinsic (i)a-Si:H interlayers are used to acheive this passivation effect. The presented work discusses the structural and electronic changes induced by low temperature post-deposition annealing of such (i)a-Si:H/c-Si structures.

The microscopic configuration of hydrogen in the thin amorphous layers, as probed by Fourier transform infrared spectroscopy (FTIRS), is linked to the improvement of the passivation and a dramatic increase of effective minority carrier lifetime τ_{eff}. With 10 nm thick undoped a-Si:H layers values up to $\tau_{\text{eff}} > 4.5$ ms, corresponding to interface recombination velocities S as low as 2 cm/s, were observed.

KR 5.3 Wed 11:00 H4

Rigorous optical simulation of rough interface light trapping structures in thin film silicon solar cells — •Daniel Lockau[1,2], Sven Burger[2,3], Lin Zschiedrich[2,3], Frank Schmidt[2,3], and Bernd Rech[1] — [1]Helmholtz–Zentrum Berlin, Berlin, Germany — [2]Zuse–Institut Berlin, Berlin, Germany — [3]JCMwave GmbH, Berlin, Germany

Thin film silicon solar cells suffer from the disadvantage of a low absorption coefficient of silicon in important spectral regions. In the case

of a flat multilayer cell layout a considerable part of the incident light is reflected back out of the cell due to the low absorber thickness. It is therefore desirable to introduce scattering elements that prolong the average photon path length inside the solar cell's absorber. Rough interfaces between the layers of a solar cell have proven to provide efficient and industrially producible light trapping structures. As the scattering structures and the layer thicknesses are in the order of only a few ten wavelengths coherence effects have to be taken into account in the simulation and optimization of such structures.

We employ the finite element method for rigorous simulation of Maxwell's equations on 2D and 3D geometries to investigate light trapping effects produced by rough interfaces in thin film silicon solar cells. To approximate an extended rough surface we examine the influence of boundary conditions and a finite computational domain size on the absorption. We apply Monte Carlo sampling over sets of surface representations to obtain averaged measurement quantities. Simulations of 2– and 3–dimensional rough surface geometries are compared.

KR 5.4 Wed 11:15 H4

Optical and structural properties of MBE grown silicon nanodots for photovoltaic application — •Maurizio Roczen, Enno Malguth, Orman Gref, and Manfred Schmidt — Helmholtz-Zentrum Berlin, Berlin, Deutschland

Third generation Solar cells are aimed to exceed the Queisser-Shockley Limit of 30 % efficiency for single junction silicon solar cells by utilizing the quantum size effect (QSE). In theory, the bandgap of nanosized silicon structures (< 5 nm) widens with decreasing size. A hetero emitter consisting of silicon nanodots embedded in a SiO_2 matrix could therefore serve as an energy selective contact allowing the extraction of high energy carriers before thermalization takes place. The SiO_2 matrix allows passivation of an adjacent c-Si absorber and of the nanodots themselves. To grow crystalline silicon nanostructures of the required size, amorphous silicon nano layers were deposited onto plasma oxidized Si-wafers and silica substrates by e-beam evaporation at ultra high vacuum. Annealing the samples above 620 °C leads to the formation of separate crystalline spheres. Both atomic force and scanning electron microscopy show a clear tendency of decreasing sphere size for thinner primal layers. Crystallinity is confirmed by Raman experiments. To observe the quantum size effect, absorption and photo luminescence measurements were carried out as well as surface photo voltage measurements to check the density of states at the interface. Recent results on doped nanodots are discussed.

KR 6: Topical Session Photovoltaic Materials II (with MM and BV MatWerk)

Time: Wednesday 11:45–13:15 Location: H4

KR 6.1 Wed 11:45 H4

The influence of reducing the chalcogen to metal ratio on phase transitions during the crystallisation of photovoltaic materials CuIn(S,Se)2 — •Astrid Hölzing[1], Roland Schurr[1], Stefan Jost[2], Jörg Palm[2], Barbara Tautz[3], Felix Oehlschläger[3], Ulrike Künecke[3], Klaus Deseler[3], Peter Wellmann[3], and Rainer Hock[1] — [1]Lehrstuhl für Kristallographie und Strukturphysik, FAU, Erlangen, Deutschland — [2]Avancis GmbH & Co. KG, München, Deutschland — [3]Materials for Electronics and Energy Technology, FAU, Erlangen, Deutschland

Time resolved monitoring of the crystallisation of the thin film absorber materials CuIn(S,Se)2 while annealing stacked elemental layers (SEL) yields phase transitions proceeding during the chalcopyrite synthesis. In-situ XRD and DSC measurements on similar processed precursors provide complementary information on intermediate phases and the reaction kinetics of the chalcopyrite formation can be obtained. Thin layers of metals and chalcogens are deposited onto Mo-coated substrates by DC-magnetron sputtering and thermal evaporation, respectively. The XRD powder diagrams recorded while annealing the SEL are quantitatively analysed by Rietveld refinements. Miscellaneous binary selenides and sulfides as well as ternary sulfoselenides are observed by the chalcogenisation of the intermetallic alloy yielding different educts for the chalcopyrite formation depending on the chalcogen content. The presented study will be focused on the influence of reducing the chalcogen to metal ratio on the processing of photovoltaic materials CuIn(S,Se)2.

KR 6.2 Wed 12:00 H4

Properties of grain boundaries in Cu(In,Ga)Se_2 and Cu(In,Ga)S_2 thin film solar cells deduced from mean inner coulomb potential measurements — •Sebastian S. Schmidt[1], Daniel Abou-Ras[1], Joachim Klaer[1], Raquel Caballero[1], Christoph T. Koch[2], Thomas Unold[1], and Hans-Werner Schock[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Max Planck Institut für Metallforschung, Heisenbergstrasse 3, 70569 Stuttgart, Germany

Polycrystalline Cu(In,Ga)Se_2 and Cu(In,Ga)S_2 thin films are efficient absorbers in thin film solar cells. The solar cell efficiencies strongly depend on the physical properties of grain boundaries in the absorbers. Here, we investigate the local behavior of the mean inner coulomb potential (MIP) at grain boundaries in Cu(In,Ga)Se_2 and Cu(In,Ga)S_2 solar cell absorbers. With in-line holography in a transmission electron microscope we measure MIP wells at grain boundaries in both types of absorber layers. The depth of the MIP wells depends on the grain boundary type as well as the composition. Generally, the potential wells have a FWHM of about 1 nm perpendicular to the plane of the grain boundary. Since the Debye length is about 10-40 nm in the absorber layers, considerable excess charge accumulations and related band bending at the analyzed grain boundaries can be excluded. A variation in composition seems to be responsible for the formation of MIP wells at grain boundaries. We discuss the local composition at grain boundaries by utilizing the isolated atom approximation.

KR 6.3 Wed 12:15 H4

Structural and chemical analyses of MOVPE-grown CuGaSe_2 layers on (001)-GaAs — •Stefanie Bierwirth[1], Susanne Siebentritt[2], Levent Gütay[2], Jes Larsen[2], and Michael Seibt[1] — [1]Universität Göttingen — [2]Université du Luxembourg

This contribution has been withdrawn.

KR 6.4 Wed 12:30 H4

Characterisation of thin C60 films using X-Ray methods — •Chris Elschner, Alexandr A. Levin, Christoph Schuenemann, Moritz Riede, and Karl Leo — TU Dresden, Institut für Angewandte Photophysik 01069 Dresden George-Bähr-Straße 1

C60 is a well known and often used molecule for state of the art organic solar cells. To increase the efficiency in these nanoscale systems, it is necessary to control the morphology of the thin film layers with the aim to optimize the electrooptical properties. Thin C60 film layers are produced via vacuum deposition under variation of substrate temperature from 30°C up to 90°C, film thickness from 25 nm to 50 nm, and vacuum chamber pressure. The characterisation of the film layers is carried out using x-ray reflection (XRR) and x-ray diffraction (XRD). From these results, the crystallinity, the film thickness, the roughness, and the density of the film layer can be estimated. Using the Scherrer equation, we estimate the average crystal size, which shows the existence of nanoscale crystals (10 nm) in a 50nm C60 film. These results are the base for the coming investigations of mixed organic layers for the use in organic solar cells.

KR 6.5 Wed 12:45 H4

Effect of film thickness, type of buffer layer, and substrate temperature on the morphology of dicyanovinyl-substituted sexithiophene films — •Alexandr A. Levin[1], Marieta Levichkova[1], Martin Pfeiffer[2], Dirk Hildebrandt[2], David Wynands[1], Chris Elschner[1], Karl Leo[1], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Heliatek GmbH, 01187 Dresden, Germany

Dicyanovinyl-substituted sexithiophenes (DCV6T) are promising photoactive materials [1]. The influence of the film thickness, type of buffer underlayer, and deposition substrate temperature on the morphology of the DCV6T layers is investigated by means of X-ray diffraction and X-ray reflectivity methods. A neat Si wafer or a Si wafer covered by a 15 nm buffer underlayer of fullerene C60 or 9,9-Bis[4-

(N,N-bis-biphenyl-4-yl-amino)phenyl]-9H-fluorene (BPAPF) is used as substrate.

The crystalline nature and ordered molecular arrangement of the films are proven down to 6 nm film thickness. With increasing substrate temperature or film thickness, the DCV6T film relaxes, resulting in reducing the interplane distances (from 11.29(5) Å to 10.78(5) Å) closer to the bulk value (10.14(1) Å). Considering the same thickness, the DCV6T film relaxes for growth on Si to BPAPF to C60. Thicker films are characterized by smaller density and higher roughness. A thin (some nm-thick) intermediate layer with linear density-gradient is formed in DCV6T/C60 interface for the films with buffer C60 layer.

[1] D. Wynands et al., J. Appl. Phys. 106 (2009) 054509.

KR 6.6 Wed 13:00 H4

Morphological study of Zinc-Phthalocyanine for organic solar cells — •Christoph Schünemann, Chris Elschner, Alexandr Levin, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, TU Dresden, Germany

Phthalocyanines (Pc) are well known organic molecules and often used in the photoactive layer of small molecule organic solar cells. Reasons for the wide application of these organic semiconductors are their thermal stability, simple way of deposition and their common use as model system. However, the influence of the morphology on the electrical properties of organic solar cells has been investigated only rudimentary so far. In this work, the crystal structure, the growth and the stacking of Zinc-Pc molecules in thin films are investigated with x-ray diffraction (XRD) and x-ray reflection (XRR) methods. For this purpose, we varied the ZnPc film thickness from 5 nm up to 50 nm and the substrate temperature while deposition from room temperature up to 90 °C. Using XRR and atomic force microscopy, we found that the roughness of ZnPc increases with increasing substrate temperature and layer thickness. The XRD measurements show that the ZnPc layers are polycrystalline for all substrate temperatures and layer thickness. Analysing the XRD pattern we also found out, that the ZnPc films are triclinic and the atomic structure does not change with variation of the deposition parameters. The dislocation density and the microstrain in the ZnPc layer decreases with rising film thickness while the crystallite size is in the range of the layer thickness.

KR 7: Topical Session Photovoltaic Materials III (with MM and BV MatWerk)

Time: Wednesday 14:45–15:45 Location: H4

KR 7.1 Wed 14:45 H4

Influence of interface preparation on minority carrier lifetime for low bandgap tandem solar cell materials — •Nadine Szabó, B. Erol Sagol, Ulf Seidel, Klaus Schwarzburg, and Thomas Hannappel — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH Hahn-Meitner-Platz 1 14109 Berlin

III-V semiconductor compounds grown by MOVPE are implemented in todays state-of-the-art third generation multi-junction solar cells. The current record multi junction solar cell grown on germanium, having Ge, Ga(In)As and GaInP as subcells, reached a record efficiency of 41.6%. The efficiency of these multi junction solar cells could be significantly increased, if its low bandgap Ge subcell would be replaced by a more efficient tandem. For this purpose the low bandgap materials InGaAs and InGaAsP are suitable. The bandgap composition of these materials allows a better yield of the solar spectrum. Based on InGaAs/InGaAsP absorber materials we have developed a low bandgap tandem solar cell with optimized bandgaps. Results of time resolved photoluminescence (TRPL) for the IR-bandgap compounds InGaAsP (1.03 eV) / InGaAs (0.73 eV) will be presented. The lifetime of minority carriers is one of the most important properties of solar cell absorber materials. We show on the example of the low band gap tandem cell how the choice of the materials, the quality of the bulk, the optimization of the band gap energies and the preparation of the critical interfaces are essential to build a high efficiency solar cell. The quality of the bulk and the preparation of the critical interfaces are essential for the growth of the double hetero structure (DHS).

KR 7.2 Wed 15:00 H4

Sulfosalt Gradient Layers for Photovoltaic Applications — •Herbert Dittrich, Dan Topa, Andreas Stadler, Johannes Stöllinger, Astrid Pachler, and Gerhard Aigner — Christian Doppler Labor ASEC, Universität Salzburg, Hellbrunner Str. 34, 5020 Salzburg, Österreich

Sulfosalts have demonstrated to be an important compound semiconductor family including more than 260 members. They are characterized by a complex chemistry and crystal structure. In this contribution the deposition of Sn-Sb-S gradient layers and their physical properties with respect to photovoltaic applications will be presented.

Sn-Sb-S gradient layers were deposited by magnetron sputtering from inhomogeneous targets on pure glass substrates and substrates covered with a Mo electrode layer as used in CIGS technology. Chemical analysis was carried out by electron microprobe analysis and results were combined in concentration maps over the substrate area. In correlation to the chemical composition, the structural aspects of the layers were measured by X-ray powder diffraction. The absorption coefficient, optical bandgap, resistivity, conduction type and the Seebeck coefficient of the sulfosalt layers were measured and, again, correlated to the chemical composition and the crystal structure.

Results will be discussed with respect to thin film solar cell applications.

KR 7.3 Wed 15:15 H4

Real-time investigations on the formation reactions in the system Cu-Sn-S — •Roland Schurr, Astrid Hölzing, and Rainer Hock — Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen-Nürnberg, Staudtstraße 3, D-91058 Erlangen

The quaternary compound kesterite Cu_2ZnSnS_4 (CZTS) is a promising candidate for the production of low-cost thin film solar cells. CZTS thin film solar cells with efficiencies of up to 6.77% were produced [1].

The understanding of the recurrent formation reactions in the system Cu-Zn-Sn-S is necessary for the optimization of CZTS absorbers and the development of low-cost thin film solar cells. In a previous publication we presented the formation of CZTS thin film solar cell absorbers from co-electroplated precursors depending on the metal ratios in the as deposited films [2]. The crystallisation of CZTS is completed by the reaction of Cu_2SnS_3 and ZnS. Further reactions mainly involved are the formation of binary and ternary Cu-Sn sulfides. Due to the phase diagrams of Olekseyuk et al. [3] of the ZnS-SnS_2 and Cu_2S-ZnS systems, the system Cu_2S-SnS_2 forms Cu-Sn sulfides at low temperatures. Real-time investigations on the formation reactions in the ternary subsystems of Cu-Zn-Sn-S while annealing stacked elemental layers provide the reaction paths of the binary and ternary sulfides.

In the present work we report on results of in-situ XRD experiments on the formation mechanisms with main focus on the Cu-Sn-S system.

[1] H. Katagiri et al., Appl. Phys. Express 1 (2008) 041201
[2] R. Schurr et al., Thin Solid Films 237 (2009) 2465
[3] I.D. Olekseyuk et al., J. Alloys Compd. 368 (2004) 135

KR 7.4 Wed 15:30 H4

Neutron diffraction investigations of kesterites: cation order and disorder — •Susan Schorr[1], Michael Tovar[2], Sergej Levcenco[3], Alexander Napetrov[3], and Ernest Arushanov[3] — [1]Free University Berlin, Institute of Geological Sciences, Germany — [2]Helmholtz Zentrum Berlin für Materialien und Energie, Germany — [3]Academy of Sciences of Moldova Republic, Institute of Applied Physics, Chisinau, Moldova

The quaternary chalcogenides Cu_2ZnSnS_4 and $Cu_2ZnSnSe_4$ have newly attracted attention as possible absorber materials in thin film solar cells.

They crystallize in the kesterite type (space group $I\bar{4}$) or stannite type structure (space group $I\bar{4}2m$), which are described as an ordered distribution of the cations on different structural sites. Cation disorder may cause site defects and hence influences the electronic properties of the material. Thus the degree of cation order/disorder plays a crucial role and was therefor in the focus of the presented investigations. A differentiation between the isoelectronic cations Cu^+ and Zn^{2+} is not possible using X-ray diffraction due to their similar scattering power. But their neutron scattering lengths are different, thus neutron diffraction opens the possibility to determine the cation distribution in these compounds. A simultaneous Rietveld analysis of neutron and X-ray powder diffraction data revealed that in dependence on the thermal

history of the samples cation disorder appears. The correlation trend between cation order/disorder and the sample growth method (solid state synthesis, Bridgemann method) will be discussed.

KR 8: Multiferroics I (Joint Session of MA, DF, KR, DS)

Time: Monday 10:15–12:45 Location: H3

Invited Talk KR 8.1 Mon 10:15 H3

Antiferromagnetic interlayer coupling in $La_{0.7}Sr_{0.3}MnO_3$ / $SrRuO_3$ superlattices — •Ionela Vrejoiu — Max Planck Institute of Microstructure Physics, Halle, Germany

Perovskite oxides are versatile materials with a broad spectrum of physical properties, such as (anti)ferromagnetism, (anti)ferroelectricity, superconductivity, and multiferroicity. As illustrating examples, $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) and $SrRuO_3$ (SRO) are both ferromagnetic perovskites with bulk ferromagnetic Curie temperatures of 370 K and 160 K, respectively. LSMO is a 3d transition metal double exchange ferromagnet, whereas SRO is a rare case of a 4d itinerant metallic ferromagnet and, in contrast to LSMO, SRO shows exceptionally strong magneto-crystalline anisotropy. Such differences make the interlayer coupling between LSMO and SRO epitaxial thin films an intriguing case. We report on LSMO / SRO superlattices (SLs) grown by pulsed-laser deposition on vicinal TiO_2-terminated $SrTiO_3$ (100) (STO) substrates. These SLs exhibit strong antiferromagnetic (AF) interlayer coupling at temperatures below 140 K, where the SRO layers become ferromagnetic. SLs in which an ultrathin nonmagnetic perovskite spacer was grown in between all the LSMO and SRO layers (so that the LSMO and SRO have no mutual interfaces) exhibited ferromagnetic coupling below 140 K. This indicates that the AF coupling occurs only in SLs with direct interfaces between LSMO and SRO. A joint study of structural characterization, SQUID magnetometry as well as first principles calculations was performed, in order to unravel the origin of this strong AF coupling.

KR 8.2 Mon 10:45 H3

Magnetic phase transition at a biferroic interface predicted from first principles — •Michael Fechner[1], Igor Maznichenko[2], Sergey Ostanin[1], Arthur Ernst[1], Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]MPI für Mikrostrukturphysik Halle, Germany — [2]Fachgruppe Theoretische Physik, Martin-Luther-Universität Halle-Wittenberg

The interface magnetoelectric effect mediates the change of the magnetization at a ferromagnetic/ferroelectric interface when the electric polarization is modified. Using first principle methods, we investigate different ultrathin ferromagnetic films (Co and Fe) on top of ferroelectric $ATiO_3$ (A=Pb,Ba) perovskites upon the occurrence of it. The calculations show that at the interface a moderately change of the size of the total magnetization takes place [1]. Further the magnetic ordering of the Fe film is sensitive to its thickness, so an unexpected antiferrimagnetic ordering appears for 2ML Fe whereas for all other thicknesses ferromagnetic ordering is preferred. Hybridization and strain effects at the interface can explain all observations. An interesting perspective for further studies will be the investigation of thin films of a CoFe alloy. This may allow gaining control of the magnetic ordering by the electric polarization.

[1] Fechner et al.. PRB 78, 212406(2008)

KR 8.3 Mon 11:00 H3

Magnetoelectric coupling at modified Fe/$BaTiO_3$ interfaces — •Martin Hölzer[1], Michael Fechner[2], Sergey Ostanin[2], and Ingrid Mertig[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg, Fachbereich Physik, D-06900 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Two-component multiferroics are gaining attention within the last years. These compound materials, consisting of ferromagnetic and ferroelectric layers, combine the advantages (e. g. high curie temperatures) of their components in a tuneable magnetoelectric structure.

Ab initio DFT studies of ultrathin Fe films on ferroelectric $BaTiO_3$ show that their magnetoelectric coupling can be enhanced considerably by means of interface alloying.

In these systems, the magnetoelectric coupling is related to structural changes in the interface region under polarisation reversal of the $BaTiO_3$ substrate. In one of the considered cases, a magnetic phase transition with high change in the total magnetization is triggered under polarization reversal.

KR 8.4 Mon 11:15 H3

Towards ferroelectric tunneling barriers with magnetic electrodes — •Daniel Pantel, Dietrich Hesse, and Marin Alexe — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

The tunneling magnetoresistance (TMR) is a well-established quantum phenomenon in oxide electronics [1]. Recently, tunneling electroresistance was experimentally investigated in an oxide ferroelectric tunneling barrier [2, 3]. Combining both functionalities in one device, i.e. a ferroelectric barrier sandwiched in between two ferromagnetic electrodes, yields interesting properties, e.g. different effects of the ferroelectric polarization on the two spin channels [4]. However, experimental results are still lacking.

In this talk we report on the growth and the properties of perovskite oxide heterostructures consisting of a pulsed laser deposition-grown thin ferroelectric barrier layer sandwiched between two magnetic electrodes. First electrical measurements on capacitor-like tunneling junctions are presented.

[1] De Teresa, J.M., *et al.*, Science **286**, 507 (1999)
[2] Contreras, J.R., *et al.*, Appl. Phys. Lett. **83**, 4595 (2003)
[3] Garcia, V., *et al.*, Nature **460**, 81 (2009)
[4] Velev, J.P., *et al.*, J. Appl. Phys. **103**, 07A701 (2008)

KR 8.5 Mon 11:30 H3

Multiferroic materials with a non-collinear spin structure - A many-particle approach — •Thomas Michael[1], Julia M. Wesselinowa[2], and Steffen Trimper[1] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Germany — [2]Department of Physics, University of Sofia, Sofia, Bulgaria

Multiferroic bulk materials with a conical spin structure are investigated in the framework of a many-particle approach. The analysis of the ferroelectric subsystem is based on a two-state quantum model. Magnetic moments interact via the Heisenberg model. The canting of the spins is incorporated by the Dzyaloshinski-Moriya interaction. A representation of the spin operators with an arbitrary quantization axis is chosen. Minimizing the free energy yields the direction of the quantization axis. The multiferroic coupling term is discussed. A Green's function technique in reciprocal space provides the temperature dependence of the magnetization, polarization and the energy of the excitations.

KR 8.6 Mon 11:45 H3

Manipulating ferroelectric domains of multiferroic $DyMnO_3$ by soft X-rays — •Victor Soltwisch, Enrico Schierle, Detlef Schmitz, Dimitri Argyriou, Fabiano Yokaichiya, Ralf Feyerherm, and Eugen Weschke — Helmholtz Zentrum Berlin

In multiferroic $DyMnO_3$, ferroelectricity is induced by cycloidal magnetic structures of a chirality coupled to the direction of the electric polarization. XRMS at the Dy-M5 resonance allows to distinguish surface regions of different chirality of the Dy-4f magnetic cycloid and, hence, can be used to image ferroelectric domains. Furthermore, the x-ray beam itself can be utilized to manipulate the distribution of domains at the crystal surface.

KR 8.7 Mon 12:00 H3

Evidence of electro-active excitation of the spin cycloid in $TbMnO_3$ — •Alexey Shuvaev[1], Viktor Travkin[2], Vsevolod Ivanov[2], Alexander Mukhin[2], and Andrei Pimenov[1] — [1]Experimentelle Physik 4, Universität Würzburg, D-97074 Würzburg, Germany — [2]General Physics Institute, Russian Academy of Science, 119991 Moscow, Russia

The coupling between the magnetic and ferroelectric orders in multiferroics is currently a topic of intense study. The materials of particular interest are those where the incommensurate cycloidal ordering of the spins drives the ferroelectricity. One of the consequences of multifer-

roicity is the existence of novel coupled magnon-phonon excitations called electromagnons. In addition to the electromagnon along the *a*-axis, the polarization analysis of the experimental spectra suggests the existence of an electro-active excitation for ac electric fields along the crystallographic *c*-axis. This excitation is possibly the electro-active eigenmode of the spin cycloid in $TbMnO_3$, which has been predicted within the inverse Dzyaloshinskii-Moriya mechanism of magnetoelectric coupling.

KR 8.8 Mon 12:15 H3

Neutron scattering studies on chiral multiferroics: magnetic structure and excitations — •T. Finger[1], M. Baum[1], A. C. Komarek[1], D. Senff[1], P. Link[6], K. Hradil[5], K. Schmalzl[4], W. Schmidt[4], L.-P. Regnault[3], D. N. Argyriou[7], P. Becker-Bohaty[2], L. Bohaty[2], and M. Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Kristallographie, Universität zu Köln — [3]CNG-Grenoble / ILL, Grenoble — [4]FZ Jülich, JCNS at ILL, Grenoble — [5]Universität Göttingen / FRM2 München — [6]FRM2, TU München, München — [7]HMI, Berlin

We present neutron-scattering experiments on IN12 and on IN14 using spherical polarization analysis directly documenting the poling of the elastic magnetic chiral terms for the spiral magnets $MnWO_4$ and $TbMnO_3$ by cooling in an electric field. In addition, we were able to observe a multiferroic hysteresis curve as function of electric field in both compounds and succeeded to switch the spiral at constant temperature, which is the central issue in view of future applications. Additionally, measurements of the diffuse scattering slightly above the multiferroic transition show some small chiral terms remaining in the collinear phase. The close coupling of ferroelectricity and magnetism in the multiferroic materials also results in new collective excitations, predicted almost 20 years ago: hybridised spin-phonon excitations, referred to as "electromagnons". After the first observations of potential electromagnon modes in infra-red and in neutron studies a conclusive interpretation is still missing. Our most recent neutron scattering measurements will be discussed.

KR 8.9 Mon 12:30 H3

Topological magnetoelectric memory effect in the spin-spiral multiferroic $MnWO_4$ — •Dennis Meier[1], Naemi Leo[1], Thomas Lottermoser[1], Petra Becker[2], Ladislav Bohatý[2], and Manfred Fiebig[1] — [1]HISKP, Universität Bonn — [2]Institut für Kristallographie, Universität zu Köln

Within the field of multiferroics, i.e. compounds with coexisting magnetic and electric order, so-called spin-spiral ferroelectrics attract tremendous attention. In these systems magnetic long-range order violates the inversion symmetry and induces a spontaneous electric polarization. Magnetic and electric domains are thus rigidly coupled so that “giant” magnetoelectric effects are obtained. However, up to now nearly nothing is know about the topology of the domain state in these systems. We report spatially-resolved measurements of the multiferroic domain topology in $MnWO_4$. For the first time, the full three-dimensional domain structure in a spin-spiral system is imaged. Our study reveals that the multiferroic domains in magnetically-induced ferroelectrics unify features that are associated to a magnetic domain state and others that point unambiguously to ferroelectric domains. Hence, a description in terms of ferroelectric or antiferromagnetic domains is incomplete and no longer appropriate. The novel concept of “multiferroic hybrid domains” is introduced. Annealing cycles reveal a topological memory effect: Due to phase coexistence at one phase boundary limiting the multiferroic state in $MnWO_4$, the entire multiferroic multidomain state can be reconstructed subsequent to quenching it. This work is supported by the DFG through SFB608.

KR 9: Multiferroics II (Joint Session of MA, DF, KR, DS)

Time: Monday 14:00–17:45 Location: H3

KR 9.1 Mon 14:00 H3

Switching of a spin-spiral-induced polarization in multiferroic $MnWO_4$ — •Tim Hoffmann[1], Dennis Meier[1], Petra Becker-Bohatý[2], Ladislav Bohatý[2], and Manfred Fiebig[1] — [1]HISKP, Universität Bonn — [2]Institut für Kristallographie, Universität zu Köln

Coexisting ferroic orders become interesting when there is an interaction between them. Especially applying an electric field and thus changing the magnetic order is highly desirable for possible applications. In spite of the declared interest in multiferroics to switch a magnetization by an electric field nothing is known about the dynamics of the actual switching process.

The coupling of ferroelectric and magnetic order is intrinsically strong in spin-spiral multiferroics, where ferroelectricity emerges as a consequence of complex magnetic long-range order. Here we observe the manipulation of magnetically-induced ferroelectric domains in $MnWO_4$ by optical second harmonic generation (SHG). Application of an electric field allows to transform the sample to an electric as well as magnetic single-domain state. Moreover we obtained images of the domain structures during the transition revealing the growth of the domains. When cooled in zero-field, the domains have a bubble-like topology. Interestingly, after recovery from a single domain state the shape changes to a stripe structure and the domain size is significantly increased. Effects of the shape and duration of the electric-field poling pulses are investigated. Furthermore, in contrast to typical ionic ferroelectrics the spontaneous polarization can be switched without fatigue – no defects or pinning effects constrain the movement of domain walls.

KR 9.2 Mon 14:15 H3

Single Crystal X-ray diffraction studies on multiferroic $YMn_{2-x}Fe_xO_5$ — •Sven Partzsch[1], Jochen Geck[1], Norman Leps[1], Roberto Kraus[1], Dmitr Souptel[1], Bernd Büchner[1], and Enrico Schierle[2] — [1]IFW Dresden — [2]Helmholz-Zentrum Berlin

Temperature dependent single crystal X-ray diffraction studies of $YMn_{2-x}Fe_xO_5$ are presented. Upon cooling, the undoped material (x=0) orders antiferromagnetically below $T_N \approx 45\,K$ and becomes multiferroic below $T_{CE} \approx 39\,K$. This multiferroic phase is destabilized rapidly with increasing Fe-content and we address here the reasons for this dramatic effect. The crystallographic study implies that the doped Fe mainly occupies the square pyramidal coordinated Mn position instead the octahedral one, which shows that these lattice sites are crucial for the MF properties.

In order to further characterize the electronic ordering in the ferroelectric phase of the undoped samples, we also applied soft resonant X-ray diffraction, which clearly shows that the oxygen states play an important role as well.

KR 9.3 Mon 14:30 H3

Electronic structure and magnetism in $YFeMnO_5$ — •Torsten Weissbach[1], Tilmann Leisegang[2], Axel Lubk[2], Dirk C. Meyer[3], and Sibylle Gemming[4] — [1]Inst. f. Theoretische Physik, TU Bergakademie Freiberg — [2]Inst. f. Strukturphysik, TU Dresden — [3]Inst. f. Experimentelle Physik, TU Bergakademie Freiberg — [4]Inst. f. Ionenstrahlphysik u. Materialforschung, Forschungszentrum Dresden

$YFeMnO_5$ crystallizes in the structure type of the orthorhombic RMn_2O_5 class of oxides. These show a series of antiferromagnetic phases with propagation vectors (1/2-δ, 0, 1/4+ϵ) below $T_N \approx 45$ K. For several of these phases, magnetism coexists with ferroelectricity. In $YFeMnO_5$, only one commensurable ferrimagnetic phase was found below $T_N = 165$ K, and ferroelectricity is absent. We apply crystallographic and quantum chemical methods to compare the Fe-substituted and the mangenese-only compounds. Diffraction experiments show slight displacements of the atom sites with increasing Fe content. The largest effects are related to crystal-field repulsion acting on the local metal 3*d* orbitals. The interaction between the magnetic metal ions is studied using DFT calculations starting with a bias magnetization of the atoms.

KR 9.4 Mon 14:45 H3

Ab initio **calculations of the magnetic properties of perovskites under deformation** — •Igor Maznichenko[1], Corina Etz[2], Arthur Ernst[2], Martin Lüders[3], Ingrid Mertig[1,2], Zdzislawa Szotek[3], and Walter Temmerman[3] — [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

Materials with perovskite and perovskite-like structures demonstrate a broad spectrum of physical properties. Colossal magnetoresistance, ferroelectricity, multiferroicity, superconductivity, charge ordering, metal-insulator transition, Jahn-Teller and other effects are observed in perovskites. These properties of the mentioned materials with the common formula ABO_3 are very sensitive to the type of the cations A and B. $La_{2/3}Sr_{1/3}MnO_3$ (LSMO) is a strongly correlated $3d$ transition metal oxide with a Curie temperature (T_C) above RT (370 K). For other La/Sr ratios different types of antiferromagnetism are observed. Other perovskite, ruthenate $SrRuO_3$ (SRO) is a $4d$ ferromagnet with $T_C = 160$ K.

Here we perform *ab initio* calculations for LSMO and SRO in ideal cubic, tetragonally distorted, and different orthorhombic structures. We focus on magnetic order and Curie temperature of the above mentioned structures in the different structural phases.

KR 9.5 Mon 15:00 H3

Electric field induced magnetization switching in strained EuO — •Marjana Ležaić, Konstantin Rushchanskii, Frank Freimuth, and Stefan Blügel — Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

EuO is one of the rare materials combining a semiconducting gap and ferromagnetic ordering. Due to this property, EuO was suggested as a spin-filter in magnetic tunnel junctions [1]. It was shown that its ordering temperature T_C of 69 K can be increased further by doping with Gd [2], or by a reduction of the lattice parameter [3]. Recently, it has also been shown that a spin-polarized 2-dimensional electron gas can be formed at the EuO/LaAlO3 interface [4]. The list of properties that are not only interesting from the point of view of basic research, but also indicate possible applications, does not end here. A newly discovered property, ferroelectricity in strained EuO [5] puts this material into the class of multiferroics with relatively high T_C. Employing *ab-initio* calculations, we demonstrate how the ferroelectric property can be exploited in EuO films under tensile strain in order to achieve electric control of the magnetization direction.

[1] T. Santos and J. S. Moodera, Phys. Rev. B **69**, 241203 (2004).
[2] R. Sutarto, *et al*, Phys. Rev. B **80**, 085308 (2009).
[3] N. J. C. Ingle and I. S. Elfimov, Phys. Rev. B **77**, 121202(R) (2008).
[4] Y. Wang, *et al*, Phys. Rev. B **79**, 212408 (2009).
[5] E. Bousquet, N. A. Spaldin, Ph. Ghosez, arXiv:0906.4235v1.

KR 9.6 Mon 15:15 H3

Ferroelectric properties of $BiFeO_3$ thin films under mechanical stress — •Martin Hoffmann, Oliver Mieth, and Lukas M. Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

Since ferroelectric properties (polarization, coercive field, etc.) of thin films can differ dramatically from the corresponding bulk values due to lattice-mismatch-induced strain, the systematic investigation of the impact of mechanical stress on the nm-length-scale is an indispensable step towards the general understanding of ferroic thin film physics.

In the present study, 150-nm-thick multiferroic $BiFeO_3$ films grown on (001)-oriented $SrTiO_3$ substrates were inspected with piezoresponse force microscopy (PFM) towards their ferroelectric domain distribution and their local ferroelectric hysteresis behavior under both tensile and compressive stress.

The systematic variation of the externally applied mechanical stress by substrate bending allowed us to compensate or to enhance the strain effect, which can be quantified by monitoring the coercive field as a function of the bending angle.

KR 9.7 Mon 15:30 H3

Strain effects in spinel ferrite thin films from first principles calculations — •Daniel Fritsch and Claude Ederer — School of Physics, Trinity College Dublin, Ireland

We present density functional theory calculations of the structural and magnetic properties of the inverse spinel systems $CoFe_2O_4$ (CFO) and $NiFe_2O_4$ (NFO). Both are insulating magnets with high magnetic ordering temperatures and large saturation magnetization, which have been of particular interest over the past few years as building blocks of multiferroic heterostructures [1]. In order to effectively design the magneto-electric response of such multiferroic heterostructures, a clear picture of strain-induced changes in the magnetic properties of CFO and NFO is particularly important. Here we present results for the structural and magnetic properties of both CFO and NFO, with special emphasis on strain-induced changes in the magnetocrystalline anisotropy energy (MAE). Our results are representative for (001)-oriented thin films of CFO and NFO, grown on different lattice-mismatched substrates. We find a large and strongly strain-dependent MAE for CFO, and a significantly smaller but also strongly strain-dependent MAE for NFO. We discuss the influence of cation order within the inverse spinel structure and analyze the effect of different exchange correlation functionals on the structural and magnetic properties.

[1] H. Zheng et al., Science 303, 661 (2004).

15 min. break

KR 9.8 Mon 16:00 H3

Mechanism of ferroelectric instabilities in non-d^0 perovskites: $LaCrO_3$ versus $CaMnO_3$ — Tim Harris, Roman Kovacik, and •Claude Ederer — School of Physics, Trinity College Dublin, Ireland

The incompatibility of partial d occupation on the perovskite B-site with the standard charge transfer mechanism for ferroelectricity has been a central paradigm in multiferroics research [1]. Nevertheless, it was recently shown by density functional theory calculations that $CaMnO_3$ exhibits a polar instability that even dominates over the octahedral tilting for slightly enlarged unit cell volume [2]. Here, we present similar calculations for $LaCrO_3$, which has the same d^3 B-site electron configuration as $CaMnO_3$. We show that $LaCrO_3$ exhibits a similar, albeit somewhat weaker, volume-dependent polar instability as $CaMnO_3$, but while the Born effective charge (BEC) for the Mn^{4+} cation in $CaMnO_3$ is highly anomalous, the BEC for Cr^{3+} in $LaCrO_3$ is only slightly enhanced. We decompose the BECs for both systems in contributions of individual Wannier functions to elucidate the different driving force behind the polar instability in these systems.

[1] N. A. Hill, J. Phys. Chem. B 104, 6694 (2000). [2] S. Bhattacharjee et al., Phys. Rev. Lett. 102, 117602 (2009).

KR 9.9 Mon 16:15 H3

Multiferroicity in $EuTiO_3$ and $Eu_{1-x}Ba_xTiO_3$: *ab initio* characterization of crystalline, magnetic and electronic structure — •Konstantin Z. Rushchanskii[1], Marjana Ležaić[1], and Nicola A. Spaldin[2] — [1]Institut für Festkörperforschung, Quanten-Theorie der Materialien, Forschungszentrum Jülich GmbH, 52425 Jülich, and JARA-FIT, Germany — [2]Materials Department, University of California, Santa Barbara, CA 93106-5050, USA

We report a systematic study of possible structural transitions in $EuTiO_3$ and ordered $Eu_{1-x}Ba_xTiO_3$ mixed compounds. We investigated phonon spectra of $EuTiO_3$ and found strong M- and R-point instabilities, indicating antiferrodistortive structural deformations. In the ordered $Eu_{0.5}Ba_{0.5}TiO_3$ compounds, the antiferrodistortive deformation is replaced by significant ferroelectric distortions, involving not only Ti, but also the magnetic Eu cation. We will discuss several scenarios of ferroelectric and antiferrodistortive transitions and their coupling with the magnetic structure. Corresponding changes in the phonon structure will be compared with available experimental data.

KR 9.10 Mon 16:30 H3

Electronic and magnetic properties of $LuFe_2O_4$ — •Karsten Kuepper[1], Michael Raekers[2], Christian Taubitz[2], Manuel Prinz[2], Christine Derks[2], Manfred Neumann[2], Andrei V. Postnikov[3], Frank M. F. de Groot[4], Cinthia Piamonteze[5], Dharmalingam Prabhakaran[6], and Stephen J. Blundell[6] — [1]Institut für Festkörperphysik, Universität Ulm, Albert-Einstein-Allee 11, D-89081 Ulm, Germany — [2]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany — [3]LPMD, Paul Verlaine University and Institute Jean Barriol, Metz, France — [4]Department of Inorganic Chemistry and Catalysis, Utrecht University, Sorbonnelaan 16, 3584 CA Utrecht, Netherlands — [5]Swiss Light Source, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [6]Department of Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford, OX1 3PU, United Kingdom

$LuFe_2O_4$ is a compound showing fascinating magneto electric coupling via charge ordering. Electronic and magnetic properties of the charge ordered phase of $LuFe_2O_4$ are investigated by means of x-ray spectroscopic and theoretical electronic structure approaches [1]. We identified the electronic states of the valence band by means of valence band XPS-, and XES-spectroscopies, and GGA+U first principles calculations. Moreover, by applying XMCD, we are able to identify the

spin ground state of $LuFe_2O_4$ in the charge ordered phase to be a 2:1 ferrimagnetic configuration, ruling out a frustrated magnetic state.

[1] K. Kuepper et al., Phys. Rev. B, Rapid Commun., in press.

KR 9.11 Mon 16:45 H3

Influence of Fe-substitution in $LiNi_{(1-x)}Fe_xPO_4$ on the antiferromagnetic structure — •Elke Künzel[1], Anne Zimmermann[1], Jiying Li[2], David Vaknin[2], and Manfred Fiebig[1] — [1]HISKP, Universität Bonn — [2]Ames Labatory and Department of Physics, Iowa States Univerity, Ames, USA

The LiMPO$_4$ system (M=Fe, Ni, Co, Mn) includes crystallographically isostructural compounds with antiferromagnetic (AFM) order differing in the spin direction only. Thus, the system offers the opportunity to study fundamental mechanisms of AFM 180° domain formation in a range of similar but not identical compounds. In spite of their structural similarity, drastic differences in the domain topology are observed by optical SHG. Domains in $LiNiPO_4$ form anisotropic platelets whereas in $LiFePO_4$ they are isotropic and amoeba-like. It is yet unclear whether this surprising behaviour is due to the properties of the nickel ion or to the spin direction which points along z in $LiNiPO_4$ and along y in $LiFePO_4$.

In order to clarify this, samples with different mixing ratios of nickel and iron were studied. The domain structure of $LiNiPO_4$ was found to become aboeba-like for an iron substitution of «50%. An anomalous temperature dependence of the AFM order parameter and indications for a spin structure different from that of the end compounds was observed.

KR 9.12 Mon 17:00 H3

Non-Resonant Magnetic X-ray Scattering on Rare-Earth Iron Borates $RFe_3(BO_3)_4$ — •Jorge E. Hamann-Borrero[1], Martin Philipp[1], Olga Kataeva[2], Martin von Zimmermann[3], Christian Hess[1], Ruediger Klingeler[1], Alexander Vasiliev[4], Leonard Bezmaternykh[5], and Bernd Buechner[1] — [1]IFW Dresden, 01171 Dresden, Germany — [2]A.E.Arbuzov Institute of Organic and Physical Chemistry of the Russian Academy of Sciences, Kazan, Russia — [3]HASYLAB at DESY, Hamburg, Germany. — [4]Low Temperature Physics department, Faculty of Physics, Moscow State University, Moscow, Russia. — [5]L.V Kirensky Institute of Physics, Russian Academy of Sciences, Krasnoyarsk, Russia.

Non-resonant magnetic XRD (NRMXRD) experiments with photon energy of 100keV where performed on selected compounds of the $RFe_3(BO_3)_4$ family as a function of temperature and applied magnetic field. The results show the existence of several unexpected diffraction features, in particular the presence of a magnetic super-lattice peak, and the appearance of two reflections that violate the diffraction conditions for the low temperature phase $P3_121$ of the iron borates. The magnetic nature of the former is concluded from analysing the scattering cross section at high energies and the magnetic structure of the different compounds. It is shown that the magnetic reflection reveals the magnetic properties of the material. For $GdFe_3(BO_3)_4$, values for the component of the spin moment perpendicular to the scattering plane ($S_\perp$) have been determined as well as the angle between the spin moment and the hexagonal basal plane.

KR 9.13 Mon 17:15 H3

Electronic structure, magnetic and dielectric properties of the edge-sharing copper-oxide chain compound NaCu2O2 — •Philippe Leininger[1], Martin Rahlenbeck[1], Markus Raichle[1], Britta Bohnenbuck[1], Andrey Malyuk[2], Chengtian Lin[1], Bernhard Keimer[1], Eugen Weschke[2], Enrico Schierle[2], Shinichiro Seki[3], Yoshi Tokura[3], and John Freeland[4] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, D-12489 Berlin, Germany — [3]University of Tokyo, Dept. of Applied Physics, Bunkyo-ku, Tokyo 113-8656, Japan — [4]Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, USA

We report an experimental study of NaCu2O2, a Mott insulator containing chains of edge-sharing CuO4 plaquettes, by polarized x-ray absorption spectroscopy (XAS), resonant magnetic x-ray scattering (RMXS), magnetic susceptibility, and pyroelectric current measurements. The XAS data show that the valence holes reside exclusively on the Cu2+ sites within the copper-oxide spin chains and populate a d-orbital polarized within the CuO4 plaquettes. Our results also demonstrate a new orbital selection rule for RMXS that is of general relevance for magnetic structure determinations by this technique. Dielectric property measurements reveal the absence of significant ferroelectric polarization below TN, which is in striking contrast to corresponding observations on the isostructural compound LiCu2O2. The results are discussed in the context of current theories of multiferroicity.

KR 9.14 Mon 17:30 H3

Magnetoelectric effect in diluted antiferromagnet $PbFe_{0.5}Nb_{0.5}O_3$ — •Vladimir Shvartsman[1], Pavel Borisov[2], Wolfgang Kleemann[2], and Antoni Kania[3] — [1]Institut für Materialwissenschaft, Fakultät für Ingenieurwissenschaften, Universität Duisburg-Essen, Essen, Germany — [2]Angewandte Physik, Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany — [3]Institute of Physics, University of Silesia, Katowice, Poland

Multiferroics, i. e. materials where two primary ferroic order parameters of magnetic and electric nature coexist, are of significant scientific and practical interest nowadays. Especially attractive are the multiferroics with enhanced magnetoelectric (ME) properties, which relate changes of polarization/magnetization to external magnetic/electric fields, respectively. While the linear ME effect has strong symmetry requirements and is rare, higher order ME couplings are allowed in all multiferroics. We report on investigations of magnetic and ME properties of (001)-oriented $PbFe_{0.5}Nb_{0.5}O_3$ (PFN) single crystals in the temperature range 5-300 K. PFN is ferroelectric below 385 K and antiferromagnetic below the Néel temperature, T_N=154 K. Temperature dependences of the magnetization exhibit a step like anomaly at T_N and a maximum on zero-field cooled curves at 8 K. Below T_N, the system manifests a spontaneous second order ME effect (electrobimagnetic effect), which reaches a peak value around 20 K. Moreover, after field cooling the linear ME effect has been observed, which disappears above 8 K. The nature of the low-temperature magnetic anomaly and the temperature dependences of the ME effects are discussed.

KR 10: Poster: Multiferroics (with MA, DF, KR, DS)

Time: Tuesday 10:45–13:45 Location: Poster A

KR 10.1 Tue 10:45 Poster A

Theorectical study of the influence of Ni-bridge-Ni angles on magnetic anisotropy and exchange — •Claudia Loose and Jens Kortus — TU-Bergakademie Freiberg, Institut for Theoretical Physics, Leipziger Str. 23, 09599 Freiberg, Germany

We studied the effect of distortions in the Ni-brigde-Ni angles of 5 small Ni-dimers by means of density functional theory calculations. In three cases we observed a decrease of the magnetic exchange coupling constant J with increasing magnetic anisotropy D. However, one of the Ni-dimers showed the opposite behaviour. The last discussed complexe displays an abrupt change from easy-axis to easy-plane as soon as one leaves the experimental geometry.

These results suggest that the development of simple guiding rules for rational design of magnetic anisotropy, similar to the well known Goodennough-Kanamori rules, may be difficult and a more detailed description based on electronic structure information may be required.

KR 10.2 Tue 10:45 Poster A

Magnetic anisotropy of paramagnetic porphyrin molecules on non-magnetic surfaces: an angle-dependent XMCD investigation — •Matthias Bernien[1], Jorge Miguel[1], Wolfgang Kuch[1], Adrian D. Ward Cherrier[2], Carsten Tieg[2], Claudia Weis[3], Carolin Antoniak[3], Dietger Bovenschen[3], and Heiko Wende[3] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — [2]ESRF, BP 220, F-38043 Grenoble Cedex, France — [3]AG Wende and Center for Nanointegration (CeNIDE), Universität Duisburg-Essen, Lotharstrasse 1, 47048 Duisburg

Metal complexes on surfaces are a topic of intensive scientific investigations since the properties of their central metal ion, determined by the adjacent ligands, can be widely tuned by the chemical de-

sign of the molecule. Here we report on the electronic structure and the magnetic properties of paramagnetic Fe and Co octaethylporphyrin molecules adsorbed on non-magnetic Cu(100) and oxygen-covered ($\sqrt{2}\times 2\sqrt{2}$)R45° O/Cu(100) surfaces. The magnetic moments of the metal centers of the molecules are aligned by an external magnetic field of 5 T at a temperature of 8 K. The magnetic anisotropy of the metal centers is probed by XMCD measurements along the easy and hard magnetization direction. For Fe porphyrin molecules on the bare Cu(100) substrate a negligible magnetic anisotropy is found. In contrast, a huge magnetic anisotropy of the Fe ion can be obtained by placing half a monolayer of atomic oxygen between the molecules and the Cu(100) surface. This work has been supported by DFG (Sfb 658 and Sfb 491) and ESRF (HE 2700).

KR 10.3 Tue 10:45 Poster A

Electron spin dynamics in novel binuclear Mn molecular complexes — •Y. Krupskaya[1], R. Zaripov[2], E. Vavilova[1,2], A. Parameswaran[1], V. Miluykov[3], I. Bezkishko[3], D. Krivolapov[3], O. Kataeva[3], O. Sinyashin[3], E. Hey-Hawkins[4], V. Voronkova[2], K. Salikhov[2], R. Klingeler[1], V. Kataev[1], and B. Büchner[1] — [1]IFW Dresden, Dresden, Germany — [2]Zavoisky Physical-Technical Institute of the RAS, Kazan, Russia — [3]A.E. Arbuzov Institute of Organic and Physical Chemistry of the RAS, Kazan, Russia — [4]Institute of Inorganic Chemistry, Leipzig University, Leipzig, Germany

We present a study of electron spin dynamics in novel Mn-dimer molecular complexes which show strong dependence of the electron density distribution at the Mn sites on the ligand surrounding. Using the pulsed electron spin resonance (ESR) technique we have detected electron spin echo and determined spin-lattice relaxation (T_1) and phase-coherence (T_2) times which systematically depend on the ligand type. Interestingly, we observe an electron spin echo envelope modulation (ESEEM) associated with the coupling of the Mn electron spins to nearby proton moments. Moreover, we show that the spin-relaxation times can be substantially increased by reducing intermolecular interactions, for instance, by dissolving the crystals in a liquid media.

KR 10.4 Tue 10:45 Poster A

Incoherent Slow Magnetisation Dynamics in the Giant Keplerat Molecule $Fe_{30}Mo_{72}$ — •T. Dellmann[1], H.-H. Klauss[1], J. Schnack[2], and B. Büchner[3] — [1]Institut für Festkörperphysik, TU Dresden — [2]Fakultät für Physik, Univ. Bielefeld — [3]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden

In the geometrically frustrated polyoxomolybdate nanomolecule $Fe_{30}Mo_{72}$ a distinct slowing down of the magnetisation dynamics is observed at temperatures of about 5K depending on the observation method [1, 2]. These dynamics still persist at very low temperatures down to 20 mK as shown by local probe techniques. Furthermore, no magnetisation steps could be found in the field dependent magnetisation at these temperatures as predicted by the quantum rotational band model [3].

We present recent low temperature ac-susceptibility results for different frequencies (200 Hz < f < 10 kHz) and external fields (0 < B < 2 T) and discuss them in comparison with results from μ^+SR, NMR and ^{57}Fe moessbauer spectroscopy. The origin of decoherence at lowest temperatures is focussed in this discussion.

[1] Chr. Schröder et al., Phys.Rev.B 77, 224409 (2008)
[2] J. Lago et al., Phys.Rev.B 76, 064432 (2007)
[3] J. Schnack et al., Europhys. Lett., 56 (6), pp. 863-869 (2001)

KR 10.5 Tue 10:45 Poster A

High-field measurements of a spin-frustrated trinuclear copper (II) complex — •Wolfgang Kroener[1], Aksana Zharkouskaya[2], Eike T. Spielberg[2], Daniel Plaul[2], Klaus Gieb[1], Winfried Plass[2], and Paul Müller[1] — [1]Department of Physics and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Germany — [2]Institut für Anorganische und Allgemeine Chemie, Universität Jena, Germany

We present magnetic measurements of a trinuclear copper II complex based on triaminoguanidin (TAG): $[Cu_3(bipy)_3(^H TAG)](ClO_4)$. A home-made micro-Hall-bar magnetometer and a commercial SQUID magnetometer were used to perform angle-resolved single crystal measurements. As the triangular structure of the complex suggests, we can conclude from our measurements, that we deal with a spin-frustrated system. Following a proposal of Trif et al.[1] we investigated the magnetization under high electric fields.

[1] M. Trif, F. Troiani, D. Stepanenko, D. Loss, Phys. Rev. Lett. 101, 217201 (2008).

KR 10.6 Tue 10:45 Poster A

Reinvestigation of the electronic and magnetic structure of the ferric star — •Daniel Taubitz[1], Karsten Kuepper[2], Rolf Saalfrank[3], Andreas Scheurer[3], Stefan Sperner[3], Jürgen Schnack[4], and Manfred Neumann[1] — [1]Department of Physics, University of Osnabrück, Barbarastrasse 7, D-49069 Osnabrück, Germany — [2]Department of Solid State Physics, University of Ulm, Albert-Einstein-Allee 11, D-89069 Ulm, Germany — [3]Institute for organic chemistry, Universität Erlangen-Nürnberg, Henkestr. 42, 91054, Erlangen, Germany — [4]Department of Physics, University of Bielefeld, Universitätsstr. 25, D-33615 Bielefeld

Large polynuclear complexes which contain transition metal and/or rare earth metal ions are of current interest due to their tunable magnetic properties and the possibility to act as single molecule magnets (SMM). The use of SMMs for information technology (e.g. molecular memory arrays) is a main target in the field of molecular spintronics. Simplest inorganic Systems, that show SMM behaviour like for example the ferric star $Fe^{III}[Fe^{III}(L^1)_2]_3$ have attracted much interest, since they can be investigated as model systems.
We investigated the ferric star with different X-ray spectroscopic techniques. The experimental results obtained by different groups using different methods will be compared and discussed.

KR 10.7 Tue 10:45 Poster A

Accuracy of the DMRG method applied to the antiferromagnetic Heisenberg icosidodecahedron — •Jörg Ummethum and Jürgen Schnack — Universität Bielefeld, Fakultät für Physik, Postfach 100131, D-33501 Bielefeld

Geometrically frustrated spin systems show a variety of fascinating properties like magnetization jumps or an enhanced magnetocaloric effect. There are many methods to study such systems like exact diagonalization, quantum Monte Carlo, or DMRG. Exact diagonalization is limited to rather small systems and quantum Monte Carlo suffers from the so-called negative sign problem. The DMRG method [1] is in principle free of such limitations but the accuracy is rather limited for systems with more than one dimension.

We present results of our DMRG studies of the antiferromagnetic Heisenberg icosidodecahedron and focus on the lowest energy levels in subspaces of total magnetic quantum number which form so-called rotational bands for many antiferromagnetic spin systems [2]. The accuracy of the results and possibilities to improve it, like different orderings of the spins, are discussed.

[1] S. R. White, Phys. Rev. B **48**, 10345 (1993)
[2] J. Schnack and M. Luban, Phys. Rev. B **63**, 014418 (2000)

KR 10.8 Tue 10:45 Poster A

DFT Studies Of A Magnetic Heptanuclear High-Spin Complex — •Stefan Leiding[1], Andrei Postnikov[2], Jürgen Schnack[1], and Dirk Andrae[1,3] — [1]Bielefeld University, Germany — [2]Paul Verlaine University Metz, France — [3]Freie Universität Berlin, Germany

The synthesis of molecular magnets has undergone rapid progress in recent years, therefore the ability to tune the couplings between the spins of individual transition metal atoms by controlled attachment of molecular ligands is examined using spin-dependent density functional theory. $[\{(talen^{t\text{-}Bu_2})\text{-}\{Mn^{III}(solv)_n\}_3\}_2\{Fe^{III}(CN)_6\}]^{3+}$ is a heptanuclear complex built via molecular recognition from three building blocks: two trinuclear manganese triplesalen units and one hexacyanometallate. In order to investigate the geometric and electronic effects on ferromagnetic coupling via the spin-polarization mechanism (well established in organic chemistry), we applied this mechanism to transition metal complexes. First of all we focus on much smaller fragments of the heptanuclear complex, e.g., the triplesalen ligand with three Mn^{III} centers and the [(N,N'-ethylenebis(salicylaldimine)) $Mn^{III}(H_2O)_2]^+$ which contains only a single Mn^{III} ion. The influence of the ligand folding in these complexes causes a change in the orientation of the magnetic orbitals and in the spin-polarizations. These properties are examined by Kohn-Sham DFT calculations with the SIESTA and the TURBOMOLE programs.

KR 10.9 Tue 10:45 Poster A

Magnetic coupling of Co porphyrin molecules to ferromagnetic substrates — •Felix Hermanns, Alexander Krüger, Matthias Bernien, Jorge Miguel, and Wofgang Kuch — Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Metalorganic compounds are promising candidates for spintronic de-

vices. In this context, the interaction of the central transition metal ion of Fe-octaethyl-porphyrin molecules with underlying ferromagnetic substrates has been studied and found that it can be changed from parallel to antiparallel [1].

Here, we report on X-ray absorption spectroscopy (XAS) measurements of submonolayers of Co-octaethyl-porphyrin on bare and oxygen-covered Ni films grown on Cu(001). By means of angle-dependent XAS measurements at the N K-edge, a parallel orientation of the quasi-planar molecule is found with respect to the surface.

The Co $L_{3,2}$ XAS and XMCD spectra display significant differences for the two substrates. Angle-dependent spectral changes are explained by the distinct contributions of the individual Co 3d orbitals. The modification of the Co oxidation state by the adsorption on the two substrates is discussed. XMCD investigations yield a ferromagnetic coupling at room temperature between the Ni substrate and the Co ion only in the case of the bare metal surface. From the temperature dependence of the Co-XMCD signal, the magnetic coupling energy is evaluated.

This work is supported by the DFG (Sfb 658).

[1] M. Bernien et al., Phys. Rev. Lett. 102, 047202 (2009)

KR 10.10 Tue 10:45 Poster A

Stability of Mn_6Cr single-molecule-magnets adsorbed on surfaces: The influence of X-ray exposure, layer thickness, choice of substrate and counterions — •Andreas Helmstedt[1], Aaron Gryzia[1], Sebastian Steppeler[1], Norbert Müller[1], Marc D. Sacher[1], Ulrich Heinzmann[1], Veronika Höke[2], Thorsten Glaser[2], Mikhail Fonin[3], and Ulrich Rüdiger[3] — [1]Fak. f. Physik, Uni Bielefeld — [2]Fak. f. Chemie, Uni Bielefeld — [3]Fak. f. Physik, Uni Konstanz

The single-molecule-magnet (SMM) Mn_6Cr consists of three main components: Two bowl-shaped Mn_3-salen complexes are bridged by a complex containing one Cr atom. Three counterions are coupled to the triply charged SMM to ensure charge neutrality. Mn_6Cr-SMM have a low stability against X-ray exposure, which adversely affects a study of the electronic properties by X-ray absorption- and photoelectron spectroscopy. With increasing exposure time, the spectral features of trivalent Mn representing intact molecules disappear while Mn(II)-typical features increase. This degradation process and its dependence on the photon flux, the substrate and the SMM concentration were observed during beamtimes at BESSY II and MAXLAB III. The rate of degradation shows also a strong dependence on the choice of counterions. The choosen preparation method allows the adsorption of Mn_6Cr-SMM with varying layer thickness on various substrates. This study reveals an influence of the substrate and the molecule layer thickness on the initial electronic state of the adsorbed molecule layer, i.e. the molecules seem to degrade already during the adsorption process.

KR 10.11 Tue 10:45 Poster A

Homogenous adsorption of Mn_6Cr single-molecule-magnets on substrates — •Peter Koop[1], Aaron Gryzia[1], Andreas Helmstedt[1], Wiebke Hachmann[1], Armin Brechling[1], Marc Sacher[1], Ulrich Heinzmann[1], Veronika Höke[2], and Thorsten Glaser[2] — [1]Molecular and Surface Physics, Bielefeld University — [2]Anorganic Chemistry I, Bielefeld University

Mn_6Cr is a single-molecule-magnet (SMM) consisting of two bowl-shaped compounds, each containing three Mn-atoms. These compounds are bound together by a Cr-complex. For charge neutrality, counterions have to be coupled to the SMM. Investigation of separated SMM, the molecule-substrate interaction and/or possible future applications e.g. data storage, requires preparation of monolayers or thin films. This preparation is done by solving Mn_6Cr in methanol, and dropping few μl of the solution onto a 9x9 mm sized substrate. Depending on the choice of substrate Au, SiO_2 (native Oxide, 50 nm Oxide), HOPG, Ru, Mn_6Cr concentration, the angle of the sample while being preparated and the amount of applied solution Mn_6Cr yields strongly varying kinds of assembly. On the one hand, clusters emerge in the solution just a moment before the solvent dries, depending on the concentration of Mn_6Cr in the solution. On the other hand the lateral distribution of the SMM is correlated with the droplet-size, the angle of the sample during preparation and the counterions, e.g. lactate anions cause Mn_6Cr to create membranes. The samples have been investigated by means of optical microscopy, SEM, surface profilometry and AFM.

KR 10.12 Tue 10:45 Poster A

Single molecule magnets on surfaces: recent advances and future perspectives — Sönke Voss[1], •Samuel Bouvron[1], Ulrich Rüdiger[1], Mikhail Fonin[1], Michael Burgert[2], and Ulrich Groth[2] — [1]Fachbereich Physik, Universität Konstanz, 78467 Konstanz — [2]Fachbereich Chemie, Universität Konstanz, 78467 Konstanz

In recent years, single molecule magnets (SMMs) have attracted much attention due to their unique properties such as quantum tunneling of magnetization (QTM) and hysteresis of pure molecular origin [1], making these materials potential candidates for future applications in ultra-high density data storage devices. Only very recently first experiments indicating the conservation of magnetic properties of SMM clusters upon surface deposition have been reported boosting the investigation of SMM monolayers [2].

We present an overview of the latest achievements in the investigation of Mn_{12} monolayers as well as the individual molecules by means of scanning probe techniques, synchrotron radiation based techniques, and magnetization measurements. In particular, novel approaches towards the assembly of Mn_{12} SMMs on substrates suited for advanced studies or possible applications are highlighted.

This work was supported by DFG through SFB 767 (TP C5).

[1] D. Gatteschi and R. Sessoli, Angew. Chem. Int. Ed. **42**, 268 (2003).

[2] M. Mannini et al., Nature Mater. **8**, 194 (2009).

KR 10.13 Tue 10:45 Poster A

Properties of TiO_2/Fe composites investigated by ab inito calculations — •Anna Grünebohm, Heike C. Herper, and Peter Entel — Fakultät für Physik, Universität Duisburg-Essen

Multiferroic materials offer interesting new applications through the coupling or coexistence of two order parameters - particularly ferroelectricity and ferromagnetism. While ferromagnetism is mainly mediated by highly localized *d*- and *f*- electrons, conventional ferroelectricity is mediated by cation off-centering which is based on empty *d*-shells. Therefore, multicomponent systems are promising alternatives for high performance multiferroics [1]. In such composites, the ferroelectric and ferromagnetic phases are coupled through hybridization and strain effects at the interfaces. To get an insight into the interface properties of such systems, we do calculations within the projector augmented wave method using VASP [2]. We investigate Fe/TiO_2 agglomerates as simple model systems in order to study fundamental properties of such interfaces. Although TiO_2 does not possess a ferroelectric phase, it offers a large polarizability and a magnetoelectric effect has been measured in Fe/$TiO_{2-\delta}$ films [3]. This means that TiO_2 interfaces possess similar properties as ferroelectrics. Until now little is konwn of the interface structure of TiO_2/Fe agglomerates. Hence, we present a systematic study of different layered systems as well as agglomerated nanoparticles.

[1] R. Ramesh and N. A. Spaldin, Nat. Mater. **6**, 21 (2007) [2] G. Kresse and J. Furthmüller, Phys. Rev. B **54**, 11169 (1996) [3] S. D. Yoon, *et al*, Appl. Phys. Lett. **92**, 042508 (2008)

KR 10.14 Tue 10:45 Poster A

Magnetism and ferroelectricity of Mn-doped $BaTiO_3$ thin films — •Yao Shuai, Danilo Bürger, Shengqiang Zhou, Manfred Helm, and Heidemarie Schmidt — Forschungszentrum Dresden-Rossendorf e.V., Bautzner Landstraße 400, 01328 Dresden

Strained $BaTiO_3$ (BTO) thin films grown by pulsed-laser deposition (PLD) on $SrTiO_3$ substrates can result in a nearly 500 K larger ferroelectric transition temperature. The remanent polarization of strained BTO thin films is at least 250% higher than that in BTO single crystals **[1]**. We used PLD to grow Mn-doped BTO (BTMO) thin films on MgO, and c-plane sapphire substrates. For example, we observed XRD reflexes of (00l)- and (l00)-oriented domains on BTMO deposited on MgO and sapphire, indicating the BTMO films are polycrystalline. At room temperature the saturated magnetic moment of BTMO films with a thickness of 400nm on MgO substrates amounted to 8 emu/cm^3, while that of the films deposited on c-sapphire was merely 1 emu/cm^3 even at 5 K, resulting from a weak domain orientation due to the large lattice mismatch between BTMO and c-sapphire. A capacitance-voltage hysteresis behavior of BTMO films on Pt/c-sapphire has been probed under a driving voltage of 50 mV at 100 kHz, which can be ascribed to the nonlinear ferroelectric response **[2]**. The simultaneously observed magnetic and ferroelectric ordering proves the feasibility of multiferroic BTMO for novel device applications**[3]**. **[1]** K. J. Choi et al., Science **306** (2004) 1005. **[2]** M. Dawber et al., Reviews of Modern Physics **77** (2005) 1083. **[3]** R. Ramesh et al., Nature Materials **6** (2007) 21. (2007) 21.

KR 10.15 Tue 10:45 Poster A

Angle-dependent magnetotransport in Nickel thin films — •M. Althammer, M. Wagner, A. Brandlmaier, M. Weiler, S. Geprägs, R. Gross, and S.T.B. Goennenwein — Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany

Angle-dependent magnetoresistance (ADMR) measurements have proven to be a powerful tool to investigate magnetic anisotropy in ferromagnetic thin films [1]. We here apply the ADMR technique to polycrystalline Nickel thin films deposited via electron beam evaporation onto $LiNbO_3$, MgO and $BaTiO_3$ substrates. The 50 nm thick films were patterned into Hall-bar structures with optical lithography and etching or lift-off. In the ADMR measurements, the longitudinal and transverse resistance is recorded as a function of the orientation of the external magnetic field at constant field strength. In all samples investigated the strain in the Nickel thin film can be tuned in situ, either via temperature or an applied electric field. Due to magnetoelastic coupling the strain leads to a change in the magnetic anisotropy. We can quantitatively explain our data with basic magnetoelastic coupling theory, taking into account the thermal dependence of the lattice parameters of the respective substrate. Fitting the data by a single domain model allows to extract the magnetic anisotropy. We also discuss the external magnetic field and temperature dependence of the resistivity parameters. Financial Support by the DFG (SPP 1157 and GO 944/3) is gratefully acknowledged.

[1] W. Limmer *et al.*, PRB **74**, 205205 (2006)

KR 10.16 Tue 10:45 Poster A

Investigation of strain effects in epitaxial $CaMnO_3$ films by nonlinear optics — •Tim Günter[1], Satadeep Bhattacharjee[2], Philippe Ghosez[2], Adrian David[3], Wilfrid Prellier[3], and Manfred Fiebig[1] — [1]HISKP, University of Bonn, Germany — [2]University of Liege, Belgium — [3]CRISMAT Laboratory, ENSICAEN, CNRS, France

The family of ABO_3 perovskite oxide compounds constitutes an important class of multifunctional materials. For $CaMnO_3$, a G-type antiferromagnetic insulator (T_N = 122 K), a weak Mn-driven ferroelectric instability at its equilibrium volume was recently predicted. Furthermore this instability can be enhanced by strain engineering, driving $CaMnO_3$ towards multiferroicity.
Here optical second harmonic generation (SHG) was used for investigating $CaMnO_3$ films grown epitaxially with 2% tensile strain on (001)-$LaAlO_3$ substrates. The temperature dependence of the SHG signal indicates a phase transition at $\approx$ 20 K with an emergence of long range order that is not found in the bulk compound. SHG polarization analysis based on SHG selection rules allows to determine the origin of this novel phase. A variety of possible ferroelectric polarization directions was considered on the basis of a symmetry analysis. First results on SHG spectroscopy and domain imaging are reported.
This work is supported by the EU-STREP MaCoMuFi.

KR 10.17 Tue 10:45 Poster A

First-principles study of ferroelectric domain walls in multiferroic bismuth ferrite — Axel Lubk[1,2], •Sibylle Gemming[3], and Nicola Spaldin[2] — [1]Institute of Physics, Technical University, D-01062 Germany. — [2]Materials Department, University of California, Santa Barbara, California 93106-5050, USA. — [3]Inst. Ion Beam Physics and Materials Research, FZ Dresden-Rossendorf, D-01314 Dresden, Germany.

The structural, electronic, and magnetic properties of the ferroelectric domain walls in multiferroic $BiFeO_3$ were studied by density-functional band-structure calculations. Domain walls in which the rotations of the oxygen octahedra do not change their phase when the polarization reorients are the most favorable and of these, the 109° domain wall centered around the BiO plane has the lowest energy. The 109° and 180° walls have a significant change in the component of their polarization perpendicular to the wall; the corresponding step in the electrostatic potential is consistent with a recent report of electrical conductivity at the domain walls. Finally, we show that changes in the Fe-O-Fe bond angles at the domain walls cause changes in the canting of the Fe magnetic moments which can enhance the local magnetization at the domain walls.
[1] Seidel et al., *Nature Mater* **8** (2009) 229; [2] Lubk et al., *Phys. Rev. B* **80** (2009) 104110.

KR 10.18 Tue 10:45 Poster A

Separation and magnetic-field dependence of contributions to the magnetically induced net polarization in multiferroic $TbMn_2O_5$ — •Naëmi Leo[1], Thomas Lottermoser[1], Dennis Meier[1], Roman V. Pisarev[2], and Manfred Fiebig[1] — [1]HISKP, Universität Bonn — [2]Ioffe Physical Technical Institute, Russian Academy of Sciences

Strong magnetoelectric coupling is expected in multiferroics in which the ferroelectric polarization is directly induced by the magnetic order. A particularly interesting magnetoelectric multiferroic is $TbMn_2O_5$, which shows a reversal of the spontaneous ferroelectric polarization P upon application of a magnetic field. Theoretical approaches predict two contributions to the net polarization directly linked to the magnetic order of the system.

The analysis of nonlinear spectra of $TbMn_2O_5$ measured by optical Second Harmonic Generation (SHG) reveals not only two but three distinct contributions P_1^{Mn}, P_2^{Mn} and P_3^{Tb}, whereas in pyroelectric measurements only the net polarization can be seen. It has been shown that the third contribution P_3^{Tb} is linked to the magnetic order of the Tb sublattice. Furthermore, spatial resolved measurements reveal additional domain structures at low temperatures.

Performing nonlinear optical measurements in an applied magnetic field reveals that the change of sign in the ferroelectric net polarization in $TbMn_2O_5$ is driven by an magnetoelectric interaction with the rare-earth order: $P(T,B) = P_1^{\mathrm{Mn}}(T) - P_2^{\mathrm{Mn}}(T,H) \pm P_3^{\mathrm{Tb}}(T,H)$. This work was supported by the DFG through SFB 608.

KR 10.19 Tue 10:45 Poster A

Influence of doping on the lattice dynamics: Comparison of stoichiometric and mixed orthorhombic rare earth manganites $RMnO_3$ (R = Gd, Tb, Eu:Y) — •S. Issing[1], F. Fuchs[1], C. Ziereis[1], E. Batke[1], A. Pimenov[1], Y. Vu. Ivanov[2], A. A. Mukhin[2], and J. Geurts[1] — [1]Physikalisches Institut, Universität Würzburg, Germany — [2]General Physics Institute of the Russian Academy of Sciences, Moscow, Russia

Among the class of multiferroics, the orthorhombic manganites $RMnO_3$ are an excellent example for the intimate coupling of lattice and magnetic degrees of freedom. For a fine tuning of the magnetic properties the isovalent substitution of the R ion can be employed leading to a quasi-continuous increase of the orthorhombic crystalline distortion and thus of the magnetic frustration responsible for multiferroicity. However the question of disorder induced by isovalent substitution needs to be adressed. Thus, employing Raman and FTIR spectroscopy, we studied the lattice dynamics of stoichiometric (R = Eu, Gd, Tb) as well as mixed $RMnO_3$ compounds ($Eu_{1-x}Y_x$ $0 \leq x \leq 0.5$ - covering the R ion radius from Eu to Tb) - to gain insight into the consequences of an isovalent partial substitution on the R-site. Our spectroscopic techniques give us sensitivity not only to symmetry properties but also to the involvement of different ion types within the unit cell. Our results clearly show that the MnO_6-octahedra remain unaffected by disorder, making $Eu_{1-x}Y_xMnO_3$ an excellent model system for a quasi-continuous fine-tuning of the lattice properties relevant for the appearance of multiferroicity.

KR 10.20 Tue 10:45 Poster A

Spin-phonon coupling in multiferroic stoichiometric and mixed $RMnO_3$ compounds (R=Gd, Tb, Eu:Y) studied by Raman spectroscopy — •S. Issing[1], A. Pimenov[1], Y. Vu. Ivanov[2], A. A. Mukhin[2], and J. Geurts[1] — [1]Physikalisches Institut, Universität Würzburg, Germany — [2]General Physics Institute of the Russian Academy of Sciences, Moscow, Russia

Spin-phonon coupling, manifesting itself as phonon softening in the temperature range of the magnetically ordered phases is investigated by temperature dependent polarized Raman spectroscopy. Stoichiometric (R = Eu, Gd, Tb) and mixed (R = $Eu_{1-x}Y_x$, $0 \leq x \leq 0.5$ - covering the R ion radius range of the stoichiometric compounds) multiferroic orthorhombic $RMnO_3$ are compared in the 10 - 300 K temperature range. The strength and temperature dependence of the phonon softening depend strongly on the mody symmetry showing the correlation of this effect with the magnetic interaction of the Mn^{3+} ions within the MnO_2-plane leading to the strongest phonon renormalization for the in-plane symmetric stretching mode ($B_{2g}(1)$). Quantitative spin-phonon coupling constants for all investigated systems are derived showing the trend of weakend spin-phonon coupling for decreasing R ion radius. Strikingly, spin-phonon coupling is observed even for $RMnO_3$ compounds with an incommensurate magnetic structure of the Mn^{3+} spins, i.e. without long-scale magnetization. This underscores the role of phonons as a quasi-local probe.

KR 10.21 Tue 10:45 Poster A

Magnetic Structure of Multiferroic $DyMnO_3$ studied by Resonant Soft X-ray Scattering — •Enrico Schierle, Victor Soltwisch, Detlef Schmitz, Ralf Feyerherm, Andrey Maljuk, Fabiano Yokaichiya, Dimitri Argyriou, and Eugen Weschke — Helmholtz-Zentrum Berlin

In multiferroic $DyMnO_3$, ferroelectricity is induced by a cycloidal magnetic structure of Mn-3d moments. However, it has been shown that ordering of Dy-4f moments strongly influences the ferroelectric properties of this compound. We examined the magnetic structure of Dy-4f moments by resonant magnetic X-ray scattering (RMXS) at the Dy-M_5 resonance in detail. As the main result, we show that over a large temperature range of the ferroelectric phase, Dy-4f moments form a magnetic cycloid of a chirality coupled to the direction of the electric polarization. This property can be exploited to map the ferroelectric domain structure at the crystal surface by RMXS.

KR 10.22 Tue 10:45 Poster A

Investigation of the triangular multiferroic order in $CuCrO_2$ by second harmonic generation — •Vera Carolus[1], Kenta Kimura[2], Tsuyoshi Kimura[2], and Manfred Fiebig[1] — [1]Helmholtz-Institut für Strahlen- und Kernphysik, Nußallee 14-16, D-53115 Bonn — [2]Devision of Materials Physics, Graduate School of Engineering Science, Osaka University, Toyonaka, Osaka 560-8531, Japan

$CuCrO_2$ (space group $R\bar{3}m$) is a triangular lattice antiferromagnet with delafossite structure showing a modulated out-of-plane 120° spin order below $T_N = 23.6$ K. Because of the breaking of inversion symmetry by the magnetic order a magnetically induced electric polarisation with six different domains should exist.

Here we investigate the multiferroic order of $CuCrO_2$ by optical second-harmonic generation (SHG) spectroscopy. Although the value of spontaneous polarisation is about four orders of magnitude weaker than in a conventional ferroelectric, a clear SHG signal with a pronounced spectral and polarization dependence is obtained. This giant coupling to the SHG progress is not restricted to $CuCrO_2$, but is also observed in $MnWO_4$, $TbMn_2O_5$ and CuO. This points to electronic instead of ionic nature of the ferroelectric polarisation.

In SHG imaging experiments the topology of the multiferroic domains (and their manipulation) were investigated. Crystallographic and magnetic correlations between the six types of domains were revealed.

KR 10.23 Tue 10:45 Poster A

Magnetic structure in multiferroic pyroxenes: (Na, Li)$FeSi_2O_6$ — •Max Baum[1], Alexander Komarek[1], Navid Qureshi[1], Petra Becker[2], Ladislav Bohatý[2], Martin Meven[3], Astrid Schneidewind[3], Peter Link[3], Maria Fernandez-Diaz[4], Paul Steffens[4], and Markus Braden[1] — [1]II. Phys. Inst., Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany — [2]Inst. für Geologie und Mineralogie, Universität zu Köln, Zülpicher Str. 49b, 50674 Köln, Germany — [3]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Lichtenbergstr. 1, 85747 Garching, Germany — [4]4 Institut Laue-Langevin, BP 156, 6 rue Jules Horowitz, 38042 Grenoble Cedex 9, France

(Na/Li)$FeSi_2O_6$ both exhibit multiferroic properties. In $NaFeSi_2O_6$ magnetic ordering is incommensurate with a temperature independent modulation k=(0, 0.23, 0). The antiferromagnetic order occurs below 8K and additionally ferroelectric ordering below 6K. Polarized neutron diffraction shows that at this transition chiral magnetic components develop. Ferroelectric order in $NaFeSi_2O_6$ seems thus to arise from the inverse Dzyaloshinski-Moriya interaction. Similarly, magnetically driven ferroelectricity is detected in $LiFeSi_2O_6$ below 18K but only at applied magnetic field. In both these compounds the electric polarization can be strongly modified by magnetic fields. Our measurement on a single crystal reveals the Shubnikov group P21/c'. On the basis of the magnetic structure we calculated the totoidal moment for $LiFeSi_2O_6$: T=-0.037muB/Å^2. This is about ten times larger than in $LiCoPO_4$, the first compound where ferrotoroidicity was unambiguously observed.

KR 10.24 Tue 10:45 Poster A

Response of antiferromagnetic and ferrotoroidic domains in $LiCoPO_4$ to magnetic and electric fields — •Anne S. Zimmemann[1], Bas B. Van Aken[1], Jean-Pierre Rivera[2], Hans Schmid[2], and Manfred Fiebig[1] — [1]HISKP, University of Bonn, Germany — [2]Department of Inorganic, Analytical and Applied Chemistry, University of Geneva, Switzerland

Ferrotoroidicity denotes a fourth form of ferroic order with a spontaneous uniform alignment of magnetic vortices. Recently the observation of antiferromagnetic (AFM) domains coexisting with ferrotoroidic (FTO) domains in $LiCoPO_4$ was reported in second harmonic generation (SHG) experiments [1]. Controlled manipulation of these FTO domains would be the next step in demonstrating the ferroic nature of the toroidal state. This could be achieved by a toroidal field, e. g. crossed electric and magnetic fields.

Here we report on the behaviour of AFM and FTO domains in external magnetic, electric, and toroidal fields. The domain structure in zero-field cooling and field-cooling experiments was investigated by SHG. Experiments showed that a magnetic field of around 5 T along the x axis changes and pins the domains. Furthermore indications for an additional phase transition were observed. Toroidal poling is thus not possible. Therefore a setup for smaller magnetic and higher electric fields was developed. - Work supported by the SFB 608.

[1] B. B. Van Aken et. al., Nature 449, 702 (2007)

KR 10.25 Tue 10:45 Poster A

Magneto-optical investigation of strain induced magnetization switching in ferromagnetic/ferroelectric hybrid structures — •Matthias Brasse[1,2], Andreas Brandlmaier[1], Matthias Opel[1], Georg Woltersdorf[3], Rudolf Gross[1], and Sebastian T. B. Goennenwein[1] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching — [2]Lehrstuhl für Physik funktionaler Schichtsysteme, Physik Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching — [3]Universität Regensburg, 93040 Regensburg

We report on the investigation of multiferroic hybrid structures, which are promising for the electric field control of the magnetization orientation. The hybrid structures consist of a ferromagnetic thin film evaporated onto a commercially available piezoelectric actuator. Making use of the piezoelectric and the magnetoelastic effect allows to control the magnetization orientation by means of the voltage applied to the piezoelectric actuator.

Spatially resolved magneto-optical Kerr effect measurements were employed to study the magnetization orientation as a function of the applied strain. Using an appropriate measurement sequence, we could demonstrate the switching of the magnetization between two distinct orientations at constant external magnetic field. We also studied local magnetization switching in the hybrid structures. Our results show, that an electric field control of ferromagnetism is possible via the elastic channel both on macroscopic as well as on microscopic scales.

This work was supported by the DFG via Go 944/3.

KR 10.26 Tue 10:45 Poster A

Giant magnetic anisotropy changes in Sr_2CrReO_6 thin films on $BaTiO_3$ — •Franz D. Czeschka, Stephan Geprägs, Matthias Opel, Sebastian T.B. Goennenwein, and Rudolf Gross — Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany

The integration of ferromagnetic and ferroelectric materials into hybrid heterostructures leads to systems with improved or even novel functionality. We here discuss the properties of the ferromagnetic double perovskite Sr_2CrReO_6, deposited as a thin film onto ferroelectric $BaTiO_3$ single crystal substrates via pulsed laser deposition. High resolution x-ray diffraction evidences the high crystalline quality of the epitaxial Sr_2CrReO_6 layers. Temperature dependent electrical transport and SQUID measurements show abrupt changes both in resistivity and magnetization at the temperatures of the $BaTiO_3$ phase transitions. Furthermore, the coercive field abruptly changes by more than 1.2 T at the $BaTiO_3$ phase transitions. These observations reveal a giant change of the magnetic anisotropy in the Sr_2CrReO_6 thin film associated with the crystalline phase transitions of the substrate. We attribute these effects to the high sensitivity of the double perovskites to mechanical deformation.

Financial support by the DFG via SPP 1157 and 1285, GO 944/3 and the Excellence Cluster "Nanoinitiative Munich" is greatfully acknowledged.

F. Czeschka et al., Appl. Phys. Lett. **95**, 062508 (2009)

KR 10.27 Tue 10:45 Poster A

Dynamics of driven multiferroic heterostructures — •Alexander Sukhov[1], Chenglong Jia[1], Paul Horley[2], and Jamal Berakdar[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Heinrich-Damerow-Str. 4, 06120 Halle/Saale, Ger-

many — [2]Centro de Fisica das Interaccoes Fundametais Instituto Superior Tecnico, Av. Rovisco Pais, 1049-001 Lisboa, Portugal

We study theoretically a ferromagnet (FM) coupled to a ferroelectric (FE) material via a multiferroic coupling. The magnetization dynamics in the ferromagnetic part is described in a standard way via the Landau-Lifshitz-Gilbert equation at finite temperatures with a dynamical driving term arising from the multiferroic coupling. Hence, an electric field that acts on the electric polarization triggers a magnetization dynamics. The ferroelectric dynamics is considered in the framework of the Landau theory of phase transitions and is governed by the Landau-Kholmogorov equation [1] augmented with a dynamical part that stems from the coupling to the ferromagnet, i.e. a magnetic field affects the polarization dynamics. We inspect how the nature of the multiferroic coupling, e.g. [2], is manifested in the time evolution of the order parameters.

[1] D. Ricinschi, C. Harnagea, C. Papusoi, L. Mitoseriu, V. Tura and M. Okuyama, J. Phys.: Condens. Matter 10, 477 (1998); [2] T. Cai, S. Ju, J. Lee, N. Sai, A. A. Demkov, Q. Niu, Z. Li, J. Shi and E. Wang, Phys. Rev. B 80, 140415(R) (2009).

KR 10.28 Tue 10:45 Poster A

Thermomechanical properties of mullite up to 1673 K: single crystal vs. ceramics — •Thomas Friedrich Krenzel[1], Jürgen Schreuer[1], and Hartmut Schneider[2] — [1]Ruhr University Bochum, Institute of Geology, Mineralogy and Geophysics, Bochum, Germany — [2]University of Cologne, Institute of Crystallography, Köln, Germany

This poster has been moved to MM 26.10.

KR 10.29 Tue 10:45 Poster A

Exchange Bias and Training Effect in Ni/Fe_xMn_{1-x}/Ni Trilayers — •Paul Stoll, Miriam Stampe, and Wolfgang Kuch — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

We have investigated ultrathin single-crystalline Ni/Fe_xMn_{1-x}/Ni/Cu(001) trilayers with out-of-plane magnetization. These trilayers show exchange bias due to the interface coupling between the ferromagnetic (FM) Ni and the antiferromagnetic (AFM) FeMn layers as well as ferromagnetic interlayer coupling between the two FM layers. Hysteresis loops for samples with different FM and AFM layer thickness and FeMn composition have been measured at different temperatures and for opposite cooling fields using polar magneto-optical Kerr effect (MOKE). The hysteresis curves show a two-step magnetization reversal with the coercivities clearly attributed to the switching fields of the two FM layers. In the minor loops unidirectional anisotropy as well as a training effect have been observed.

Financial support by the DFG (KU1115/9-1) is acknowledged.

KR 10.30 Tue 10:45 Poster A

Relative orientation of the magnetic moments in the Fe/MnPd exchange bias system — •S. Brück[1,3], S. Macke[1], X. Ji[2], Q. Zhan[2], K. M. Krishnan[2], and E. Goering[1] — [1]Max-Planck-Institut für Metallforschung, Stuttgart, Germany — [2]Department of Materials Science and Engineering, University of Washington, Seattle, USA — [3]Physikalisches Institut, Universität Würzburg, Würzburg, Germany

Recent soft X-ray resonant magnetic reflectometry (XRMR) investigations of a Fe/MnPd exchange bias system have revealed a complex magnetic configuration at the ferromagnet (F)/antiferromagnet (AF) interface in the system[1]. The existence of a considerable amount of rotatable uncompensated magnetic moments in the antiferromagnet as well as the confinement of pinned uncompensated moments to the F|AF interface was shown. Precise knowledge of the location and relative orientations of all kinds of magnetic moments at the F|AF interface is a necessary prerequisite for the development of new models for the description of exchange bias. We show how by comparing the signs and magnitudes of the absorptive part of the index of refraction, it is possible to determine the relative coupling directions in the system. It is found that rotatable Mn and the ferromagnetic Fe couple antiparallel. The pinned Mn moments are oriented antiparallel to the neighboring rotatable Mn and parallel with respect to the Fe during the field cooling process.

[1] S. Brück, G. Schütz, E. Goering, X. Ji, and K. M. Krishnan, Phys. Rev. Lett. 101, 126402-4 (2008).

KR 10.31 Tue 10:45 Poster A

Investigation of exchange bias field of NiMn pinned Co nanoparticles — •Balati Kuerbanjiang, Benjamin Riedmüller, and Ulrich Herr — Institut für Mikro- und Nanomaterialien, Universität Ulm, 89081, Ulm, Germany

Co nanoparticles deposited on a sputtered NiMn layer have been studied for the purpose of the exchange bias field. About 30 nm of NiMn layer was deposited on Si substrate by magnetron sputtering, then Co nanoparticles were deposited in situ on the NiMn layer using inert gas condensation technique. Samples were subsequently covered by about 5 nm of Cu in order to prevent oxidation of particles in air. Chemical states and compositions of the samples were examined by XPS inside the UHV system. Ex situ annealing has been carried out to achieve the antiferromagnetic NiMn phase at 350 °C for 10 min, in an applied field of 350 Oe. Annealing was performed under vacuum to avoid degradation of the magnetic properties. The phase transformation of the NiMn was investigated by X-ray diffraction. The size and the coverage of Co nanoparticles has been determined by AFM and SEM. The influence of the magnetic interaction between NiMn AFM layer and the FM Co particles of different sizes and densities was studied using vibrating sample magnetometry (VSM), magneto-optical Kerr effect (MOKE) and magnetic force microscopy (MFM).

KR 10.32 Tue 10:45 Poster A

Long and short term changes of the exchange bias field in MnIr/CoFe bilayers after ion bombardment with 10keV He ions — •Christoph Schmidt, Jörn Burbank, Niklas Stein, Tanja Weis, Dieter Engel, and Arno Ehresmann — Department of Physics, University of Kassel, Heinrich-Plett-Str.40, D-34132 Kassel

The stability and time dependence of the exchange bias (EB) field after 10 keV He^+ ion bombardment (IB) were studied. The long term measurements were done ex-situ in a time window between half an hour and several weeks after IB and the short term measurements in-situ between a few seconds and half an hour after IB. The following changes were observed: (i) the long term changes have a logarithmic behaviour of the EB field to larger values while (ii) the short term investigations show an exponential decrease of the EB field and a relaxation back to its origin direction of the unidirectional anisotropy. The two different behaviours depend on the time scale of the measurements after IB.

KR 10.33 Tue 10:45 Poster A

Remote control of superparamagnetic nanobeads on magnetically patterned thin films — •Daniel Lengemann, Tanja Weis, Alla Albrecht, Jannick Langfahl-Klabes, Dieter Engel, and Arno Ehresmann — University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

He-ion bombardment were used to get a periodic magnetic patterning with alternating anisotropy directions in exchange biased MnIr/CoFe thin layers. In remanence superparamagnetic nanobeads were located at the domain walls where the strong stray fields reach their maximum. Within an external inhomogeneous magnetic field it is possible to saturate the sample, i.e. the periodic magnetic patterning and therewith the stray fields vanish and the nanobeads can follow the gradient of the field. This mechanism allows a controlled movement of the nanobeads. First results are shown.

KR 10.34 Tue 10:45 Poster A

Coercivity mechanism in hard magnetic $SmCo_5$/$PrCo_5$ bilayers — •Felix Fleischhauer, Volker Neu, and Ludwig Schultz — IFW Dresden, Institute of Metallic Materials, 01069 Dresden, Germany

The evolution of the coercivity in hard magnetic $SmCo_5$/$PrCo_5$ bilayers shows a non-trivial dependence on the relative sublayer thickness and the stacking order.

These dependencies have been studied for bilayers with 40 nm overall thickness. They were epitaxially grown on Cr buffered MgO(110) substrates using pulsed laser deposition technique. Temperature dependent coercivity was measured in the range from 200 K to 400 K along with the magnetic relaxation at room temperature. The results are discussed within the framework of several pinning concepts.

KR 10.35 Tue 10:45 Poster A

Single or multichannel Kondo effect in graphene — •Zhen-Gang Zhu[1], Kai-He Ding[2], and Jamal Berakdar[1] — [1]Institut für Physik, Martin-Luther Universität Halle-Wittenberg, Heinrich-Damerow-Straße 4 06120 Halle, Germany — [2]Department of Physics and Electronic Science, Changsha University of Science and Technol-

ogy, Changsha 410076, China

Dynamic screening in a Kondo system may compensate or over compensate for the localized magnetic moment signifying respectively a Fermi or a non-Fermi liquid ground state. The former (latter) case occurs in one (two) channel Kondo effect with a magnetic impurity having spin 1/2. We investigate this issue in graphene starting from the tight-binding Anderson model. Schrieffer-Wolff transformation is performed to derive the Kondo model. To verify our findings, we also conduct direct computations by considering the two-body interaction explicitly. At last, the Kondo temperature is calculated from Anderson model in the large U limit. We find: i) for nearest neighbor hopping, a two-channel Kondo character is present when the impurity is symmetrically coupled to the A and B sublattice; otherwise a single channel Kondo is realized. ii) The exchange interaction coefficient for one channel is vanishing when the spin is symmetrically coupled to the spanned sublattice to this channel in absence of a gate voltage. However it is finite in the presence of a gate voltage. iii) The degeneracy of the two Dirac points leads only to a higher Kondo temperature which is increasing exponentially with increasing gate voltage. We point out the experimental feasibility by varying a gate voltage.

KR 10.36 Tue 10:45 Poster A

Magnetotransport measurements on Heusler compounds — •A. Krupp[1], F.D. Czeschka[1], M. Althammer[1], S.T.B. Goennenwein[1], R. Gross[1], I.-M. Imort[2], G. Reiss[2], and A. Thomas[2] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Fakultät für Physik, Universität Bielefeld, Bielefeld, Germany

Magnetic anisotropy (MA) is of fundamental importance in ferromagnets, as it strongly influences their properties. Using magnetotransport measurements, we investigate the MA of the Heusler compound Co_2FeAl. A 20 nm thick Co_2FeAl film on (001)-oriented MgO substrate was patterned into Hall-bar mesa structures with optical lithography and etching. The anisotropic magnetoresistance (AMR) is then measured with the external magnetic field applied in the film plane. The measured longitudinal and transverse resistance show a clear field dependence with distinct steps at small external magnetic fields ($\mu_0 H$), indicating abrupt switching of the magnetization orientation. To quantify the MA, we record the angle dependent magnetoresistance (ADMR), i.e. the MR as a function of *H-orientation* for different magnetic field magnitudes $|H|$. From the ADMR data taken at high $|H|$, AMR coefficients are obtained. The MA is then extracted from ADMR at lower $|H|$. We obtain a cubic MA field of around $\mu_0 H_{\mathrm{cub}}$=5 mT and an uniaxial MA field of around $\mu_0 H_{\mathrm{uni}}$=1 mT. We also discuss the evolution of MA with temperature and compare our results to literature.

KR 10.37 Tue 10:45 Poster A

Anomalous Hall Effect in Heusler Compounds — •I.-M. Imort[1], G. Reiss[1], A. Thomas[1], A. Krupp[2], F.D. Czeschka[2], M. Althammer[2], R. Gross[2], and S.T.B. Goennenwein[2] — [1]Fakultät für Physik, Universität Bielefeld, Bielefeld, Germany — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany

The anomalous Hall Effect (AHE) is a fundamental but still controversially discussed phenomenon in ferromagnets. Furthermore, it is a volatile characterization tool for magnetic materials. We here report on our magnetotransport experiments and the AHE in the Heusler compound Co_2FeAl. Using rf-magnetron sputtering, 20 nm thick Co_2FeAl thin films were grown on single-crystal MgO(001) substrates. Before patterning into 80μm wide Hall bars, some of the samples were annealed at different temperatures. The Hall resistivity ρ_{xy} and the magnetoresistivity ρ_{xx} were measured simultaneously over a temperature range of 3 to 300 K and a magnetic field range of $|14|$ T. For low magnetic fields $\mu_0 H$, ρ_{xx} exhibits typical anisotropic magnetoresistance features, with resistance jumps and a non-linear dependence on H. This behaviour abruptly changes at higher fields: for $\mu_0 H \geq 1.6$ T, ρ_{xx} scales strictly linearly with H. In contrast, the Hall resistivity always is proportional to $|H|$, but the slope of ρ_{xy} abruptly changes sign at $\mu_0 H \approx 1.6$ T. We will discuss the impact of temperature, surface roughness and annealing temperature on the magnetotransport properties and compare our results to the literature.

KR 10.38 Tue 10:45 Poster A

Annealing time and temperature dependence of structural, magnetic and transport properties of Co2MnSi-based MTJs — •Hendrik Wulfmeier, Markus Meinert, Daniel Ebke, Jan Schmalhorst, and Günter Reiss — Bielefeld University, Thin Films and Physics of Nanostructures, Department of Physics, Universitätsstr. 25, D-33615 Bielefeld, Germany

A high tunnel magnetoresistance effect (TMR) in magnetic tunnel junctions (MTJs) is the key for developing new spinelectronic devices like MRAM or magnetic sensors.

Optimization of MTJ-stacks where at least one electrode is built of a Heusler-alloy has been topic of many studies in recent time.

In order to enhance the level of crystallinity post-annealing is very successful. In general this effect is limited by interdiffusion processes at the interfaces of the individual layers. Crystallization and interdiffusion are both time- and temperature-dependent processes.

In our study we investigated not only the effect of different annealing temperatures but also the influence of different annealing times on the crystal structure and on the electronic properties. We prepared half (Co2MnSi | MgO) and full (Co2MnSi | MgO | CoFe | MnIr) MTJs on MgO[001]-substrates by sputter deposition and used x-ray diffractometry, MOKE and standard transport measurements for characterization.

The comparison of the experimental results (structural, magnetic and transport properties) will be discussed.

KR 10.39 Tue 10:45 Poster A

Magnetic transport measurements of epitaxial $SmCo_5$ in pulsed magnetic fields — •Evelyn Stilp, Alexander Kauffmann, Marietta Seifert, Jens Freudenberger, Volker Neu, Nadejda Kozlova, and Ludwig Schultz — IFW Dresden, Institute for Metallic Materials, Helmholtzstr. 20, 01069 Dresden, Germany

$SmCo_5$ is a hard ferromagnetic material with a high Curie temperature around 800°C and a high coercivity of 3T. With the help of a Quantum Design PPMS vibrating sample magnetometer magnetic properties were already measured. Hence an anisotropy field of 28T was calculated [1]. The epitaxial $SmCo_5$ thin films were prepared by pulsed laser deposition on Cr buffered MgO(110) [2]. Hall measurements of $SmCo_5$ thin films will be presented.

[1] A. Singh *et al.*, Phys. Rev. B 77, 104443 (2008)
[2] A. Singh and V. Neu *et al.*, J. Appl. Phys. 99, 08E917 (2006)

KR 10.40 Tue 10:45 Poster A

Epitaxial $NdCo_5$/$SmCo_5$ bilayers — •Marietta Seifert, Ludwig Schultz, and Volker Neu — IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany

$RECo_5$ magnets are of interest due to their strong magnetocrystalline anisotropies, which in some cases change with temperature. This work presents epitaxial $NdCo_5$/$SmCo_5$ bilayers, in which $NdCo_5$ undergoes a spin reorientation transition from easy axis along the *c*-axis above 310 K to easy plane below 255 K while $SmCo_5$ keeps the uniaxial anisotropy in the whole temperature range. The films were prepared on Cr buffered MgO(110) substrates resulting in a growth of the $RECo_5$ with a single orientation of the *c*-axis parallel to the film plane. In a first step, the magnetic behavior of single $NdCo_5$ thin films have been investigated and it was found that they possess intrinsic magnetic properties and especially a spin reorientation transition in good agreement with single crystal data. To analyze the magnetic coupling of the bilayer system, a series with a fixed thickness of the $SmCo_5$ layer and a varying thickness of the $NdCo_5$ have been prepared. Phase formation and texture were controlled with XRD and texture measurements. The magnetic properties in a temperature range between 20 and 400 K have been measured with Vibrating Sample Magnetometry.

KR 10.41 Tue 10:45 Poster A

Remanence enhancement and energy density in epitaxial exchange-coupled $SmCo_5$/Fe-Multilayers — •Simon Sawatzki, Felix Fleischhauer, Marietta Seifert, Ludwig Schultz, and Volker Neu — IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, D-01071 Dresden, Germany

Exchange-coupled $SmCo_5$/Fe-multilayers have been epitaxially grown by pulsed laser deposition on Cr covered MgO(110) substrates, such that one single in-plane easy axis of the highly anisotropic $SmCo_5$ phase is realized through the whole layer stack. The phase formation and texture was confirmed by Bragg-Brentano X-ray diffraction and pole figure measurements. The magnetic properties were characterized by vibrating sample magnetometry. In order to maximize the energy density $(BH)_{\mathrm{max}}$, as a key property for permanent magnet application, two series of samples were investigated. First, trilayers of $SmCo_5$/Fe/$SmCo_5$ with fixed $SmCo_5$ layer thickness (25 nm) and varying soft magnetic Fe film thickness have been prepared to analyze

the impact of the Fe-volume fraction on remanence enhancement and coupling. In the second series $SmCo_5$/Fe alternating multilayer with constant Fe-volume fraction but reduzed single layer thickness were examined.

KR 10.42 Tue 10:45 Poster A

Epitaxial $NbFe_2$ thin films prepared by PLD — •Andreas Reisner, Silvia Haindl, Bernhard Holzapfel, and Ludwig Schultz — IFW Dresden, Institute of Metallic Materials, 01069 Dresden, Germany

The hexagonal Laves phase $NbFe_2$ shows an interesting itinerant magnetic behaviour whose ferromagnetic transition at low temperatures is strongly dependent on the stochiometry.

We report on successful preparation of epitaxial thin films grown on single crystalline Al_2O_3 (001) substrates by an UHV pulsed laser deposition process. Structural investigation show a twofold epitaxial relation of $Al_2O_3(001)[100]||NbFe_2(001)[100]$ and $Al_2O_3(001)[100]||NbFe_2(001)[210]$. Magnetic and transport properties of films with various compositions near the stochiometric point have been investigated.

KR 10.43 Tue 10:45 Poster A

In-Situ STM, LEED and MOKE Measurements of Ultrathin Epitaxially Flat Grown Fe Films on the GaAs(110) Surface — •Tim Iffländer, Martin Wenderoth, Thomas Druga, and Rainer G. Ulbrich — IV. Physikalisches Institut, Georg-August-Universität Göttingen

Fe films of up to 8 ML thickness were deposited on cleaved n-, p- and i-GaAs(110) in a two-step process combining low-temperature deposition at 130 K with a subsequent annealing to room temperature. Low-energy electron diffraction and scanning tunnelling microscopy suggest an abrupt interface without any considerable amount of compound formation and a flat continuous morphology with height variations in the monolayer range.

In-situ longitudinal magneto-optical Kerr effect measurements at RT were conducted for different in-plane orientations of the applied magnetic field with respect to the sample. In contrast to RT grown Fe films of 2-3 ML thickness, the easy and hard axes are interchanged, now parallel to the [001] and [110] directions, respectively. The hysteresis loop of films thicker than or equal to 5 ML is equivalent to magnetization curves observed in the case of RT grown films.

This work was supported by the SFB 602 TP A7.

KR 10.44 Tue 10:45 Poster A

Magnetic and structural investigations of iron based nanostructures and thin CrSb layers on GaAs(110) — •Carsten Godde, Sani Noor, Atena Rastgoo Lahrood, Gregor Nowak, Hartmut Zabel, and Ulrich Köhler — Institut für Experimentalphysik IV, Ruhr-Universität Bochum, Germany

In this contribution we present structural and magnetic measurements of the two different systems, Fe and CrSb layers on the GaAs(110) surfaces.

We investigate the growth of Fe on the GaAs(110) surface at different coverages and annealing temperatures by STM and MOKE and show that the structure remains ferromagnetic up to 500°C in combination with lateral structuring on the nanometer scale. These nanostructures consist exclusively of roof-shaped 3D-islands elongated along the $[1\bar{1}0]$-direction of the GaAs(110) substrate. An intermixing of the Fe film and the substrate material induced by the annealing step leads to a ternary alloy $Fe_3Ga_{2-x}As_x$ which is confirmed by X-ray diffraction measurements. Despite of this alloying it should be noted that the magnetic measurements of the nanostructures still show ferromagnetic characteristics.

Thin CrSb layers grow in the zinc blende structure and contrary to the Fe system they keep their ferromagnetic properties and structural stability up to very high annealing temperatures which is interesting for enabling better crystalline quality. In this context the CrSb layers were characterised by STM, LEED and SQUID magnetometry at different coverages and annealing temperatures.

KR 10.45 Tue 10:45 Poster A

Structural and magnetic investigations of Fe and Fe_3Si as CEO-grown spin aligning layers on spin LEDs — •Sani Noor[1], Carsten Godde[1], Hasmik Harutyunyan[1], Arne Ludwig[2], Mingyuan Li[3], Gregor Nowak[1], Dirk Reuter[2], Martin Hofmann[3], Hartmut Zabel[1], Andreas Wieck[2], and Ulrich Köhler[1] — [1]Experimentalphysik IV, Ruhr-Universität Bochum — [2]Angewandte Festkörperphysik, Ruhr-Universität Bochum — [3]Photonik und Terahertztechnologie, Ruhr-Universität Bochum

We focus on the the structural and magnetic properties of Fe and Fe/MgO as spin injection layers on the GaAs(110) cleaved edge of spin LEDs. Within the scope of our work, we have developed an in situ process to cleave the sample within a μm range of the designated edge and deposit the layers. We show a MOKE study of the magnetization behaviour in the case of Fe which forms a Schottky barrier on n-GaAs and Fe with an MgO interlayer as a tunnelling barrier as a function of the layer thickness. STM images of Fe grown on μm-wide terraces of the cleaved GaAs(110) surface are also presented. Finally, we discuss the results of electroluminescence measurements to determine the efficiency of spin injection across the cleaved edge.

We furthermore present an STM growth study of Fe_3Si/GaAs which as a Heusler alloy is also a possible candidate as a spin aligner. In contrast to Fe/GaAs we find layer-by-layer growth even above RT. Epitaxial and stoichiometrical quality has been confirmed by XRD and LEED. Our angular dependent in situ MOKE measurements show that the Fe_3Si/GaAs(001) system exhibits only a weak magnetic anisotropy.

KR 10.46 Tue 10:45 Poster A

Threshold photoemission magnetic circular dichroism at the spin reorientation transition of ultrathin epitaxial Pt/Co/Pt(111)/W(110) films — •Kerstin Hild, Jakob Emmel, Gerd Schönhense, and Hans-Joachim Elmers — Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany

We report on the thickness dependence of threshold photoemission magnetic circular dichroism (TPMCD [1]) in one-and two-photon photoemission (1PPE and 2PPE) for a Pt-capped ultrathin Co wedge grown on Pt(111)/W(110) using femtosecond laser light. TPMCD measurements result in asymmetries continuously increasing with the sample thickness. This indicates that the TPMCD asymmetry is dominantly influenced by the Co bulk properties. At 5 monolayers (ML) asymmetry values of 0.07 % for 1PPE and 0.11 % for 2PPE are derived. The spin reorientation transition is detected at a Co thickness of 5.5 ML. For the perpendicularly saturated sample the TPMCD does not depend on the orientation of the easy axis. The comparison of the 2PPE TPMCD asymmetries with measured Kerr ellipticities in the framework of the Jones formalism reveals considerable differences between both quantities.

Funded by DFG (EL 172/15-1), the Carl-Zeiss-Stiftung and the Graduate School of Excellence MAINZ (Kerstin Hild). [1] K. Hild et al., J. Phys.: Condens. Matter 20, 235218 (2008).

KR 10.47 Tue 10:45 Poster A

Magnetization reversal and reorientation in $DyCo_5$ systems — •Radu Abrudan[1], Ilie Radu[2], Detlef Schmitz[3], Hartmut Zabel[1], and Florin Radu[3] — [1]Experimentalphysik IV, Ruhr-Universität Bochum, 44780 Bochum, Germany — [2]Institute for Molecules and Materials, Radboud University Nijmegen, 6525 ED Nijmegen, The Netherlands — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany

$DyCo_5$ is a ferrimagnet which develops a compensation point (CP) at low temperatures where the magnetic structure switches 180 degrees, a spin reorientation (SR) point at a temperature higher then room temperature, where the magnetisation axis of Dy and Co drops in plane, parallel to the substrate.

We present a systematic study of sputter deposited $DyCo_5$ thin films using XMCD technique in a transmission geometry. The spin and orbital magnetic moments of Co and Dy exhibit a monotonous temperature dependence. The ferrimagnetic alignment between the Dy and Co moments is preserved across both phase transitions, occurring at the spin reorientation (T_{SR} ∼350 K) and at the compensation (T_{CP} ∼120K) temperatures, respectively. Notably, the magnetic crystalline anisotropy changes orientation from in-plane at high temperatures to out-of-plane below T_{SR}. At T_{CP} the coercive field is strongly enhanced, diverging in size due to the reduced averaged magnetization specific to ferrimagnetic systems. Moreover, the orientation of the magnetic moments of Dy and Co reverses sign when crossing the T_{CP}.

KR 10.48 Tue 10:45 Poster A

Transition from shape anisotropy to magnetocrystalline anisotropy in ultrathin FePt films — •Karin Leistner, Juliane Wunderwald, Sebastian Fähler, and Ludwig Schultz — IFW Dresden, Dresden, Germany

FePt films have recently attracted great interest as possible media for perpendicular magnetic recording, but also for fundamental studies of magnetism in reduced dimensions. As FePt it is very corrosion resistant it is ideal for ultrathin films, however, L10 ordering and thus high magnetocrystalline anisotropy are harder to achieve at small particle size. In the present study, 2 nm thick FePt films have been deposited by pulsed laser deposition on MgO(001) with a Cr/Pt buffer. The magnetic properties have been obtained by Hall measurements and measurements of the Kerr rotation. Without post annealing, the out-of-plane (op) hysteresis is controlled by shape anisotropy with an anisotropy field of 1.4 T. The easy axis lies in-plane and in the op hysteresis curve rotation of magnetization is observed. This is as expected for smooth ultrathin disordered FePt films. When post annealing is applied, a continuous decrease of the effective in-plane anisotropy field is observed with increased annealing time. After a post annealing time of 15 min, the easy axis lies op and the op hysteresis shows switching of magnetization and a larger coercivity. The reason is that ordering in the (001)-textured films leads to an increased magnetocrystalline anisotropy in the op direction that competes with shape anisotropy. Thus, in these ultrathin FePt films anisotropy can be continuously adjusted from pure shape anisotropy to magnetocrystalline anisotropy.

KR 10.49 Tue 10:45 Poster A

Design and preparation of substrates with perpendicular magnetic anisotropy for molecular magnets — •Jonathan Fetting[1], Jan-Philipp Grote[1], Michael Stocker[2], Michael Enzelsberger[2], Veronika Höke[3], Carl-Georg Frhr. v. Richthofen[3], Paul Müller[2], Thorsten Glaser[3], and Günter Reiss[1] — [1]Bielefeld University, Department of Thin Films and Physics of Nanostructures, Universitätsstr. 25, 33615 Bielefeld — [2]University Erlangen-Nürnberg Physikalisches Institut III, Erwin-Rommel-Str. 1, 91058 Erlangen — [3]Bielefeld University, Department of Inorganic Chemistry, Universitätsstr. 25, 33615 Bielefeld

In spintronics thin films with out of plane magnetization are highly desirable for, e.g., electrodes in tunnelling cells or substrates for molecular magnets. The goal of our work is to be able to define desired film properties and to tailor the thin films correspondingly. For our approach we have chosen $[CoPd]_X$ as hard magnetic and $[CoAu]_X$ as soft magnetic multilayers. Mixing those multilayer systems gives the possibility to design the material properties. The multilayer systems have been prepared using sputter deposition techniques and the resulting thin films have been investigated with AGM, STM and MFM. The measurements give an insight into the structural and magnetic properties of the tailored samples and improve the ability to property design.

KR 10.50 Tue 10:45 Poster A

Imaging of magnetic coupling in trilayerd microstructures — •Julia Kurde[1], Jorge Miguel[1], Daniela Bayer[2], Jaime Sánchez-Barriga[3], Logane Tati Bismaths[3], Martin Aeschlimann[2], Hermann A. Dürr[3], and Wolfgang Kuch[1] — [1]Freie Universität Berlin — [2]Technische Universität Kaiserslautern — [3]Helmholtz-Zentrum Berlin für Materialien und Energie

Magnetic properties of microstructures consisting of either an FeNi single layer or an FeNi/Cu/Co trilayered system were investigated by means of photoelectron emission microscopy. We performed stroboscopic pump-probe experiments to determine the precession frequencies and the effective field of the FeNi layer. From the comparison of these measurements to micromagnetic simulations, the coupling field in the trilayered systems could be extracted. This information can then be used to explain the observed domain wall (DW) configurations in the FeNi layer. The parallel coupling of the two magnetic layers via the non-magnetic spacer layer is dominated by Néel coupling. However, the strong stray field of the DWs in the Co layer forces the magnetization to align antiparallel in the two layers, and so to turn with opposite sense of rotation from domain to domain. In 180° walls, a left turn is symmetric to a right turn, but in 90° walls of the Co layer, this will lead to a 270° turn of the magnetization in the FeNi layer. Although this case is highly unfavorable with respect to the exchange interaction within the FeNi layer, it still occurs if the Cu spacer layer reduces sufficiently the Néel coupling to the Co layer.

This work has been supported by the BMBF 05 KS7 KE2

KR 10.51 Tue 10:45 Poster A

Magnetostrictive Strain Sensors Based on FeGa Thin Films — •Ahmed Fazir Thajudin, Dirk Meyners, and Eckhard Quandt — Chair for Inorganic Functional Materials, Institute for Materials Science, Faculty of Engineering, University of Kiel, Kaiserstr. 2, 24143 Kiel, Germany

Tunneling magnetoresistance junctions generally possess a symmetrical characteristic which reflects the switching fields of the soft and hard layers, respectively. This characteristic can be changed by a stress field if the soft magnetic layer is replaced by a suitable magnetostrictive layer. Application of mechanical stress results in a stress induced rotation of the magnetostrictive layer with respect to the reference layer accompanied by a resistance change due to the magnetoresistance effect. Highly sensitive strain sensors with CoFeB electrodes based on this concept were developed recently [1]. Further increase of sensitivity is expected by the introduction of highly magnetostrictive FeGa layers. The magnetic and magnetostrictive properties of magnetron sputtered FeGa thin films are discussed. Moreover, tunneling magnetoresistance stacks with FeGa sensing layers were prepared, patterned by optical lithography and investigated with respect to microstructure, effect amplitude and magnetic switching behavior.

[1] D. Meyners, T. von Hofe, M. Vieth, M. Rührig, S. Schmitt, and E. Quandt, J. Appl. Phys. 105, 07C914, 2009

KR 10.52 Tue 10:45 Poster A

Influence of strain on magnetic and electrical properties of La0.82Sr0.18CoO3 films — •Orkidia Bilani-Zeneli, Diana Rata, Andreas Herklotz, Ludwig Schultz, and Kathrin Dörr — IFW Dresden, Institute for Metallic Materials, Helmholtzstrasse 20, 01069 Dresden, Germany

Cobaltite perovskites La(1-x)Sr(x)CoO3 have received attention mainly due to the thermally driven spin state transitions of the Co ions. For different doping, these transitions have been shown to be sensitive towards pressure in bulk and epitaxial strain in thin films. La(1-x)Sr(x)CoO3 with x=0.18 is of particular interest because it is located near the boundary of the Metal-Insulator transition. We have grown epitaxial La0.82Sr0.18CoO3 (LSCO) thin films by pulsed laser deposition on different substrates (PMN-PT, LaAlO3, SrTiO3, LSAT) providing reversible and static strain. In this work the influence of biaxial strain on the magnetic and electrical transport properties of LSCO films will be presented. Thin films reveal significant differences in magnetic behaviour with respect to bulk, e.g. the coercive fields are strongly enhanced. On the other hand tensile strain strongly suppresses the electrical conduction stabilizing thus an insulator state.

KR 10.53 Tue 10:45 Poster A

Specular and off-specular scattering of neutrons from Si-Fe multilayers — •Anke Teichert, Thomas Krist, Jan E. Hoffmann, Amitesh Paul, and Roland Steitz — Helmholtz Zentrum Berlin, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Multilayers (ML) are used as neutron optical devices. These applications require high quality MLs with low interface layer thickness, roughness and high remanence as characterized by a high reflectivity and high polarization efficiency. Here, we want to produce high quality stress-free Si-Fe MLs on Si and glass substrate. All samples (10(10nm Si+10nm Fe)+10nm Si) were produced in a triode sputter machine at p=0.065Pa and Bias voltages from 10 to 65V. Stress and reflectivity measurements were performed at a profilometer and X-ray reflectometer (XRR). Using polarized neutron reflectometry (PNR) and a positive sensitive detector (PSD) at the reflectometer V6 we measured simultaneously specular and off-specular scattering of neutrons. We find a raise in voltage leads to linear decrease of tensile stress with a slope of 5.5MPa/V. At about 60V the samples are nearly stress-free. The grain size decreased with higher Bias voltage. The off-specular data show large diffuse scattering from all samples at low applied magnetic fields (200G, 20G) as well as for samples with high compressive stress at 1030G. It appears as streaks perpendicular to specular reflectivity at Bragg peak positions. They can be interpreted as originating from vertically correlated in-plane magnetic domains. Associated longitudinal fluctuations produce additional diffuse streaks along Bragg peak positions which are independent of the stress within the samples.

KR 10.54 Tue 10:45 Poster A

Soft x-ray magnetic dichroism of undoped, hole-doped and electron-doped $LaCoO_3$: Anisotropies and valence-dependent magnetism — •Michael Merz[1], Christian Pinta[1,2], Andrei Samartsev[1,2], Markus Wissinger[1,2], Hilbert von Löhneysen[1,2], Andrea Assmann[1,2], Stephan Uebe[1,2], Dirk Fuchs[1], Peter Nagel[1], and Stefan Schuppler[1] — [1]Karlsruhe Institute of Technology, Institut für Festkörperphysik, Germany — [2]Karlsruhe Institute

of Technology, Physikalisches Institut, Germany

Epitaxial thin films of undoped $LaCoO_3$, of electron-doped (La,Ce)CoO_3, and of hole-doped (La,Sr)CoO_3 exhibit ferromagnetic order with optimum transition temperatures of 80 K, 30 K, and 240 K, respectively. The spin-state structure for these compounds was studied by soft x-ray absorption and magnetic circular dichroism at the Co $L_{2,3}$ and O K edges. It turns out that for epitaxial $LaCoO_3$, strain imposed by the substrate preserves a higher spin state of the Co^{3+} ions at low temperature and prevents a non-magnetic ground state. For (La,Ce)CoO_3, the Co^{3+} ions are predominantly in a low-spin (S = 0) state and thus magnetically inactive, and the ferromagnetism is determined by the Co^{2+} species. For (La,Sr)CoO_3, on the other hand, the magnetism originates from higher spin states of Co^{3+} (S = 2) and Co^{4+} (S = 3/2) ions. The data show that ferromagnetism has a different origin in $LaCoO_3$ (superexchange), (La,Ce)CoO_3 (spin blockade), and (La,Sr)CoO_3 (double exchange). Moreover, a strong magnetic anisotropy is observed for all systems, with the spin and the orbital moments essentially lying within the substrate plane.

KR 10.55 Tue 10:45 Poster A

Soft x-ray magnetic dichroism of (Ca,Sr)RuO_3: Evidence for strain-dependent magnetism — •Andrea Assmann[1,2], Stephan Uebe[1,2], Michael Merz[1], Markus Wissinger[1,2], Hilbert von Löhneysen[1,2], Dirk Fuchs[1], Peter Nagel[1], and Stefan Schuppler[1] — [1]Karlsruhe Institute of Technology, Institut für Festkörperphysik, Germany — [2]Karlsruhe Institute of Technology, Physikalisches Institut, Germany

The 4d transition metal oxide $Ca_{1-x}Sr_xRuO_3$ exhibits ferromagnetic order in the doping range $0.4 \lesssim x \lesssim 1$ while it is a paramagnetic metal for $x \lesssim 0.4$. Since $Ca_{1-x}Sr_xRuO_3$ remains essentially isostructural and has a similar electronic configuration throughout the doping series, the differences in the magnetic properties might be caused by chemical pressure or magnetic dilution. To verify a possible dependence of the magnetic moments on pressure, (Ca,Sr)RuO_3 films were deposited on different substrates (LSAT, STO, $DyScO_3$=DSO), with the lattice mismatch imposing a specific strain on the epitaxial films that increases when going from LSAT to STO and DSO. The magnetic and electronic structure of the strained samples was studied by soft x-ray absorption and magnetic circular dichroism at the Ru $M_{2,3}$ and O K edges. It turns out that at 20 K, the magnetic moments strongly depend on the strain: while the spin moment of samples on LSAT almost vanishes, a distinct moment is found for (Ca,Sr)RuO_3 films deposited on STO and DSO. Furthermore, a significant magnetic anisotropy is observed, with the spin moments mainly oriented perpendicular to the substrate plane. Implications will be discussed.

KR 10.56 Tue 10:45 Poster A

Vector MOKE analysis on ultrathin ferromagnetic films — •Timo Kuschel[1], Hauke Bardenhagen[1], Robin Schubert[1], Henrik Wilkens[1], Daniel Bruns[1], Martin Suendorf[1], Bernd Zimmermann[1], Florian Bertram[2], and Joachim Wollschläger[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany — [2]HASYLAB at DESY, Notkestr. 85, 22607 Hamburg, Germany

In order to study the magnetic reversal and the magnetic anisotropy of ultrathin ferromagnetic films, Fe layers of different thicknesses are assembled on MgO(001) substrates by Molecular Beam Epitaxy (MBE) under UHV conditions. The films are capped by amorphous silicon to avoid oxidation after leaving the UHV chamber. The structural characterization including X-Ray Reflectivity (XRR) and X-Ray Diffraction (XRD) measurements are performed at HASYLAB (DESY, Hamburg).

The vector MOKE analysis is based on measurements using parallel and perpendicular polarized light as well as external magnetic fields parallel and perpendicular to the incident plane of light to optain the components of the magnetization vector. A self-programmed tool is used for analyzing the magnetization curves and calculating the magnetization vector for the reversal process of different sample directions.

The results reveal a 180° reversal with a domain splitting involved for the external magnetic field parallel to one of the magnetic easy axis of the sample. The data for the magnetic hard axis show a rotation of the magnetization vector into the magnetic easy axis followed by a 90° reversal and subsequent rotation into the magnetic hard axis back.

KR 10.57 Tue 10:45 Poster A

Quadrupol-Magnetometer für breitbandige Magneto-Optische-Kerr-Spektroskopie — •Marc Tesch[1], Markus Gilbert[1], Hans-Christoph Mertins[1], Roman Adam[2], Herbert Feilbach[2] und Claus Michael Schneider[2] — [1]FH Münster, Stegerwaldstr. 39, 48565 Steinfurt — [2]FZ Jülich, IFF-9, 52425 Jülich

Üblicherweise nutzen Polarimetrieexperimente Laserlicht mit wenigen festen Wellenlängen. Die vorgestellte Polarimetrie-Anlage arbeitet mit einer Entladungsbogenlampe im Spektralbereich von 230nm - 1000nm. Sie ermöglicht Messungen des Faraday- und des Kerr-Effekts wobei ein neuartiges mit FeNdB Permanentmagneten arbeitendes Quadrupol-Magnetometer homogene Magnetfelder von bis zu 570mT in longitudinaler oder transversaler Geometrie erzeugt. Eine Wasserkühlung des inzwischen zum Patent angemeldeten Gerätes ist nicht erforderlich, was einen leichteren Einsatz im UHV ermöglicht. Die Funktionalität der Anlage wird anhand von Reflexions- und Polarisationsmessungen an dünnen Co Einfach- und Mehrfachschichtsystemen demonstriert und eine Verstärkung des Kerr-Effektes durch Interferenzeffekte diskutiert.

KR 10.58 Tue 10:45 Poster A

Magnetically Induced Optical Nonlinearity in the Centrosymmetric Ferromagnetic Semiconductor EuO — •Masakazu Matsubara[1], Andreas Schmehl[2], Jochen Mannhart[2], Darrell Schlom[3], and Manfred Fiebig[1] — [1]HISKP, Universität Bonn, Germany — [2]Institut für Physik, Universität Augsburg, Germany — [3]Department of Materials Science and Engineering, Pennsylvania State University, USA

EuO is a magnetic semiconductor, which undergoes a ferromagnetic transition at the Curie temperature (T_C) of 69 K. This material exhibits some extreme properties such as a huge colossal magnetoresistance (CMR) effect, the largest magneto-optical effect for any material, and nearly 100% spin polarization of the charge carriers in the ferromagnetic state. These outstanding properties make EuO a very attractive candidate for the basic and applied science of spintronics.

Here we report about the linear and nonlinear optical properties in epitaxial EuO, into which oxygen vacancies are introduced, grown on a $YAlO_3$ substrate. Even though EuO has a centrosymmetric crystal structure, second-harmonic generation (SHG) was observed below T_C at the two-photon transition energies from the 4f to the 5d states of Eu^{2+}. The results of the temperature and magnetic field dependent measurements suggest a close correlation between SHG and magnetization. The symmetry analysis provides access to the microscopic origin of this magnetically induced SHG signal.

This work was supported by the Alexander von Humboldt Foundation.

KR 10.59 Tue 10:45 Poster A

Interaction of surface acoustic waves with magnetization dynamics — •Rupert Huber[1], Mathias Weiler[2], Sebastian T.B. Goennenwein[2], Sebastian Neusser[1], and Dirk Grundler[1] — [1]Lehrstuhl für Physik funktionaler Schichtsysteme, Technische Universität München, Physik Department, James-Franck-Str. 1, 85747 Garching b. München, Germany — [2]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meissner-Strasse 8, 85748 Garching b. München, Germany

The authors investigate the transmission of surface acoustic waves (SAWs) in the GHz regime through thin ferromagnetic films (FM) deposited on a $LiNbO_3$ substrate. We use e.g. Co and FeCoV. When applying an in-plane magnetic field $\vec{H}$ under different orientations we find characteristic angular dependencies of the SAW's amplitude and phase on $\vec{H}$. We discuss our observation in terms of the magnetic field dependent change of elastic properties of the FM/$LiNbO_3$ hybrid systems. The dependencies are investigated in detail by comparing FeCoV and Co. FeCoV is magnetically isotropic, whereas Co shows a pronounced magnetic anisotropy. We find a significant difference for the SAW transmission characteristics. The work has been supported by the German Excellence Cluster "Nanosystems Initiative Munich".

KR 10.60 Tue 10:45 Poster A

Phenomenology of the magnetic shape memory effect in modulated and non-modulated Ni-Mn-Ga and FePd alloys — •Aristide T. Onisan and Ulrich K. Rössler — IFW Dresden

Large magnetic shape memory effects in ferromagnetic martensites are observed only in modulated phases, but recently such effects are also demonstrated in the non-modulated (NM) phase of Ni-Mn-Ga with tetragonal crystal structure and $c/a > 1$. The modulated structures have been identified with adaptive, ultra-finely twinned martensite structures of the same tetragonal structure [1]. We develop a phenomenological theory of magnetic martensites based on geometric con-

tinuum theory of martensites, linear elasticity, and micromagnetism [2]. A cubic to tetragonal martensitic transition underlies the twinned microstructures, and magnetic anisotropy is modelled by easy-axis or easy-plane uniaxial anisotropy with four-fold in-plane anisotropy. Equilibrium phase diagrams for the distribution of crystallographic variants and magnetic domains are calculated in dependence on external magnetic fields and stresses. Applications are presented for the easy-axis system with materials parameters for 5M-type Ni_2MnGa, and for FePd and NM Ni_2MnGa as easy-plane systems. Modulated phases like 5M are constructed by second-order twinning within the concept of adaptive martensites [1]. Their magnetic properties depend on the relation between magnetic exchange length and modulation period.

[1] S. Kaufmann et al., arXiv:0906.5365. [2] A.N. Bogdanov, A. DeSimone, S. Müller, U.K. Rößler, J. Magn. Magn. Mater. 261 (2003) 204-209. Supported by DFG, SPP 1239.

KR 10.61 Tue 10:45 Poster A

Surface structure and electronic properties of epitaxial off-stoichiometric Ni-Mn-Ga films — •Aleksej Laptev[1], Philipp Leicht[1], Mikhail Fonin[1], Yuansu Luo[2], Konrad Samwer[2], Yuriy Dedkov[3], and Martin Weser[3] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz — [2]I. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin

Ni_2MnGa alloys have attracted considerable interest due to the large magnetic field-induced strain and their possible applications as microscale actuators or sensors. Upon cooling from the austenite phase a transformation to the martensite phase occurs for these materials. Here we report on the investigation of epitaxial off-stoichiometric Ni-Mn-Ga films grown on MgO substrates by dc-magnetron sputtering. To achieve appropriate surface quality the samples were treated under ultra high vacuum conditions by repeated cycles of sputtering and annealing. The crystal structure changes at the Ni-Mn-Ga (100) surface during the reversible phase transition were followed by LEED. A splitting of the main reflexes due to a longer range ordering of the surface was observed upon cooling. The twin boundary formation together with the modulation of the structure was imaged by high resolution STM in the martensite phase. Electronic properties were investigated by ultra-violet photoemission spectroscopy showing pronounced differences in the valence band spectra of two phases. Financial support by the BMBF within MSM-Sens 13N10061 and 13N10062 is gratefully acknowledged.

KR 10.62 Tue 10:45 Poster A

In vitro study of iron-palladium ferromagnetic shape-memory alloy in simulated body fluid (SBF) — •Yanhong Ma, Florian Szillat, and Stefan G. Mayr — Leibniz-Institut fuer Oberflaechenmodifizierung, Translationszentrum fuer regenerative Medizin und Fakultaet fuer Physik und Geowissenschaften der Universitaet Leipzig, Permoserstrasse 15, 04318 Leipzig

Ferromagnetic shape memory alloys are a special class of active materials. They exhibit large actuation strain in martensitic phase due to a magnetic field induced reorientation of twin variants. For their biomedical applications, the biocompatibility is very important, as e.g. indicated by simulated body fluid (SBF) test. In the present study we focus on biocompatibility of $Fe_{70}Pd_{30}$ thin films. The surface morphologies and composition of the samples were studied by scanning electron microscopy equipped with energy dispersive X-ray spectroscopy. Analysis of the thin films crystalline structure was performed by X-ray diffraction. The elemental concentrations in SBF were measured after the samples were removed, using inductively coupled plasma optical emission spectroscopy. SBF experiments show that when the samples were immersed into the solution for 48 hours, some changes on the elemental concentration in SBF occurred. The Fe concentration in the as prepared SBF was about 0.002 mg/ml and no Pd was detected. After the sample was soaked into the solution for two days, concentrations of 0.028 mg/ml(Fe) and $<$0.001 mg/ml (Pd), respectively, were determined. This indicates, that some Fe moved into the solution from the film while the concentration of Pd did not change during the test.

KR 10.63 Tue 10:45 Poster A

Origin of the tetragonal distortion in Fe-Pd shape memory alloys — •Ingo Opahle[1], Klaus Koepernik[2], Ulrike Nitzsche[2], and Manuel Richter[2] — [1]Institut für Theoretische Physik, Universität Frankfurt, 60438 Frankfurt/Main, Germany — [2]IFW Dresden, P.O.B. 270016, D-01171 Dresden, Germany

Magnetic shape memory alloys (MSMA) have attracted considerable attention as materials for actuator and sensor applications, due to large magnetically induced strains of up to 10%. A promising MSMA is disordered $Fe_{70}Pd_{30}$ with an induced strain of about 6% and a relatively high blocking stress.

We have calculated the electronic structure of disordered Fe-Pd alloys [1] in the framework of density functional theory using the full potential local orbital (FPLO) code. The origin of the tetragonal distortion in these completely disordered alloys is found to be a Jahn-Teller like effect, which allows the system to reduce its band energy in a narrow composition range. In this composition range, the energy landscape along the Bain path is found to be flat, in agreement with a large tunability of strain observed in epitaxial films, covering most of the Bain path from fcc to bcc [2]. On the basis of our results, we discuss the prospects for an optimization of the alloys' properties by adding third elements, including effects on the magneto-crystalline anisotropy energy.

[1] I. Opahle *et al.*, Appl. Phys. Lett. 94 (2009) 072508.
[2] J. Buschbeck *et al.*, Phys. Rev. Lett. 103 (2009) 216101.

KR 10.64 Tue 10:45 Poster A

Herstellung und magnetische Charakterisierung von Co-Nanopartikel auf ionenstrahlerodierten Siliziumsubstraten — •Matthias Buhl, Michael Körner, Monika Fritzsche, Ullrich Wiesenhütter, Oskar Liedke und Jürgen Fassbender — Forschungszentrum Dresden - Rossendorf e.V., Dresden, Deustschland

Co-Nanopartikel wurden auf den selbstorganisierten Ripplen ionenstrahlerodierter Si-Substrate mittels Molekularstrahlepitaxie deponiert. Im Rahmen der Untersuchung sind Substrattemperatur und nominelle Beschichtungsdicke gezielt variiert worden. Mit Hilfe der longitudinalen magneto-optischen Kerr-Effekt Magnetometrie wurde der Einfluss der Ripple-Oberfläche auf das magnetische Verhalten der Co-Partikel analysiert. Die Auswertung der Messergebnisse von normierter remaneter Kerr-Drehung θ_r/θ_s und Koerzitivfeldstärke H_c zeigt eine kleine uniaxiale magnetische Anisotropie. Die leichte Richtung der Magnetisierbarkeit liegt parallel zu den Ripple-Wellenfronten.

KR 10.65 Tue 10:45 Poster A

Characterization of bioinspired synthesized magnetic nanoparticles — •Annalena Wolff[1], Katrin Eckstädt[1], Dieter Akemeier[1], Inga Ennen[1], Irina Dück[1], Katrin Wollschläger[2], Norbert Sewald[2], and Andreas Hütten[1] — [1]Department of Physics, University of Bielefeld, Germany — [2]Department of Chemistry, University of Bielefeld, Germany

Size distribution, morphology and magnetization of nanoparticles are important properties in many applications. In this study Cobalt Ferrite nanocrystals were synthesized using a biomineralization protein containing 25 amino acids and oxidative coprecipitation of Co^{2+} and Fe^{2+}. An AGM was used for magnetization measurements. A FIB DualBeam System was used to examine the morphology and size distribution. Furthermore the morphology and size distribution of chemically produced CoAu nanoparticles was examined with the DualBeam System and the magnetization with an AGM. Previously GMR was succesfully measured on CoRuNanoparticles structures. Now GMR was measured of a setup consisting of two gold contacts which are connected through a structured monolayer of CoAu nanoparticles. GMR was measured at room temperature and at low temperatures. Two point measurements and four point geometry measurements on single particle are planned.

KR 10.66 Tue 10:45 Poster A

MOKE investigation of ferromagnetic nanoparticles deposited on a W(110) surface — •Christian Kleinhans[1], Wolfgang Rosellen[1], Volker Hückelkamp[1], Furkan Bulut[1,2], Joachim Bansmann[2], Armin Kleibert[3], and Mathias Getzlaff[1] — [1]Institute of Applied Physics, University of Düsseldorf, Germany — [2]Department of Surface Chemistry, Ulm University, Germany — [3]Swiss Light Source at the Paul Scherrer Institute, Villigen, Switzerland

Magnetic properties of supported 3d-metal nanoparticles, differing from the behaviour of bulk material, open the possibility of applications from a technological point of view. With a continuously working, UHV-compatible arc cluster ion source (ACIS), ferromagnetic nanoparticles have been produced and subsequently mass filtered using an electrostatic quadrupole-deflector-unit, ensuring sizes of 5 to 15 nm. The deposition of these preformed free particles onto a W(110)-substrate is performed under soft-landing conditions. Their size and

shape is determined by means of STM and TEM. Applying a magnetic field in plane of the sample with variable angle, the magnetic behaviour of the nanoparticles is characterised using magneto-optical Kerr effect (MOKE). The influence of the angle and strength of the magnetic field on the magnetization is used to determine the nanoparticles' magnetic anisotropy and correlate this characteristic property with the respective structural behaviour.

KR 10.67 Tue 10:45 Poster A

Temperaturabhängige Magnetrelaxometrie an magnetischen Nanopartikeln aus Magnetit im Temperaturbereich von 4,2 K bis 320 K — •Markus Schiffler[1], Markus Büttner[1], Peter Weber[1], Paul Seidel[1], Claus Lang[2], Dirk Schüler[2] und Michael Röder[3] — [1]Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik — [2]Ludwig-Maximilians-Universität München, Bereich Mikrobiologie — [3]INNOVENT e.V. Jena

Obwohl Magnetit das älteste bekannte magnetische Material und seit vielen Jahren Gegenstand intensiver Untersuchungen ist sind die Ursachen vieler Eigenschaften noch nicht abschließend geklärt. Es wurden magnetische Nanopartikel aus einkristallinem Magnetit, die vom Bakterium Magnetospirillum gryphiswaldense erzeugt worden sind, mit Hilfe der temperaturabhängigen Magnetrelaxometrie (TMRX) untersucht. Dabei wird das Signal der magnetischen Relaxation der Probe mit einem axialen SQUID-Gradiometer zweiter Ordnung (Arbeitstemperatur 4,2 K) detektiert. Die Probentemperatur kann dabei durch einen entsprechenden Antikryostaten im Bereich von 4,2 K bis 320 K variiert werden. Bei der Untersuchung der Magnetitpartikel wurden Relaxationssignale in verschiedenen Temperaturbereichen und mit verschiedenen Ursachen gefunden. Die Néelrelaxation liefert einen Beitrag bei Temperaturen ab 300 K. Im Temperaturbereich des für Magnetit bekannten Verwey-Übergangen bei 110 K liegen ebenfalls signifikante Signale vor, deren Herkunft bei TMRX-Messungen erklärbar ist. Zusätzlich existieren Signale zwischen 4,2 K und 70 K, die auf eine Relaxation magnetischer Momente hindeuten.

KR 10.68 Tue 10:45 Poster A

Oxidation of multilayers of ligand stabilized magnetic cobalt nanoparticles — •Britta Vogel[1], Axel Dreyer[1,2], Nadine Mill[1], Katrin Eckstädt[1], Annalena Wolff[1], Dieter Akemeier[1], Alexander Weddemann[1], Alexander Auge[1], Simone Herth[1], and Andreas Hütten[1] — [1]Department of Physics, University of Bielefeld, D-33615 Bielefeld, Germany — [2]Department of Chemistry, University of Bielefeld, D-33615 Bielefeld, Germany

Cobalt nanoparticles have been prepared with TOPO, subsequently a ligand exchange was carried out. Samples have been prepared by dropping particle solution on Si-wafer, which lead to samples which consist of multilayers partially. The samples were studied with respect to the 3D order to gain information about the influence of the ligand on the 3D structure of the particle array and the oxidation process in multilayered particles.

KR 10.69 Tue 10:45 Poster A

Interplay between magnetism, structure and chemical order in small CoPt clusters: Ab initio and model calculations — •Lucila Juárez-Reyes, Jesus Dorantes-Dávila, and Gustavo Pastor — Institut für Theoretische Physik, Universität Kassel, Germany

The magnetic properties of small Co_NPt_M clusters ($N + M \leq 5$) are studied using a generalized gradient approximation to the density functional theory (DFT) and a self-consistent tight-binding (SCTB) model. First, we perform a systematic study of all posible different topological geometries, spin-moment configurations and chemical orders in the framework of the DFT. Second, by using the optimal ab initio structures we determine the spin moments, orbital moments and magnetic anisotropy energy within the SCTB method. The DFT calculations yield compact structures with particularly short bond lengths among the Co atoms ($d_{Co-Co} \simeq 2.2 - 2.4$Å). Pt doping induces an important enhancement of the Co spin moments μ_{Co} which are about $0.25\mu_B$ larger than μ_{Co} in Co_N. This is mainly due to important charge transfers between the Co and Pt atoms. SCTB calculations show a 15–20 % orbital contibution to the total magnetic moment. Finally, a non trivial dependence of the MAE landscape on Pt concentration is observed.

KR 10.70 Tue 10:45 Poster A

First principles study of segregation and interface effects in magnetic CoRh nanoparticles — •Luis Enrique Diaz Sanchez, Jesus Dorantes Davila, and Gustavo Pastor — Institut für Theoretische Physik, Universität Kassel, Heinrich Plett. Str. 40, 34132 Kassel, Germany

The magnetic properties for Co_xRh_{1-x} nanoparticles in the size range $N \simeq 50 - 250$ atoms are investigated in the framework of density functional theory for concentrations $x = 0.0, 0.25, 0.5, 0.75$, and 1.0. CoRh clusters are found to be magnetic with an average spin moment per Co atom that is larger than in macroscopic alloys with similar concentrations. Results are given for the local and average spin moments, charge distribution, and density of electronic states for different types of segregation (e.g., core-shell, wetting, and non-wetting), interface mixing, and random alloys. The theoretical findings are discussed by comparison with available experiments.

KR 10.71 Tue 10:45 Poster A

Magnetic properties of CoRh core shell nanoparticles — •Björn Münzing[1], Kai Fauth[1], Nabil Atamena[2], Diana Ciuculescu[2], and Catherine Amiens[2] — [1]Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]LCC Toulouse, 205 rte. de Narbonne, 31077 Toulouse Cedex 04, France

We present an X-ray magnetic circular dichroism (XMCD) study of the magnetic properties of Co@Rh core-shell-nanoparticles with a mean diameter of ≈ 1.8 nm, prepared by colloidal chemistry using organometallic precursors.

The local Co atomic magnetic moments in particles of different composition increase with increasing amount of Rh. This may be attributed to a decreasing influence of tetramethylpiperidine ligands on the 3d-metal when the particle surface is enriched with Rh. The magnetic response is essentially superparamagnetic ($T \geq 12$ K) and magnetic saturation is not attained in applied fields of up to 3 T for all compositions. The measurement of the magnetic circular dichroism on Rhodium reveals the ferromagnetic coupling of Co and Rh in these particles.

Additionally we find striking differences in magnetic coupling between the particles at short inter particle distance. This could be attributed to an effective antiferromagnetic coupling once the particle surfaces are significantly enriched with Rh.

KR 10.72 Tue 10:45 Poster A

Resistive switching in nanocolumnar manganite thin films structured with e-beam lithography — •Christin Kalkert, Markus Esseling, Jon-Olaf Krisponeit, Vasily Moshnyaga, Bernd Damaschke, and Konrad Samwer — I. Phys. Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Manganites show an intriguing variety of different behavior such as the colossal magnetoresistance, the colossal electroresistance and a resisitive switching phenomenon. Changing the resistance as a function of external parameters such as a magnetic or electric field has the potential of creating non-volatile memory applications.

In this work we studied $La_{0.7}Sr_{0.3}MnO_3$ thin films prepared by metal-organic aerosol deposition technique on Al_2O_3 substrates. The films show columnar nanostructure as determined from X-ray diffraction and TEM measurements. After macroscopic electronic and magnetic characterisation we structured the films to μm-sized bridges by means of electron beam lithography. The current voltage dependances measured at 5 K indicate tunneling mechanism of conductivity and show resistive switching between low and high resistive states. The discussion is based on local structural changes at the grain boundaries.

This work is supported by DFG via SFB 602, TP A2 and the Leibniz Program.

KR 10.73 Tue 10:45 Poster A

Magnetoresistrance of thin film microstructures of the Heusler compounds Cu_2MnAl and Co_2MnSi — •Mohamed Obaida[1,2], Denise Erb[2], Kurt Westerholt[2], and Hartmut Zabel[2] — [1]Institut für Experimentalphysik 4,Ruhr-Universität Bochum,44780 Bochum — [2]National Research Center, Tahrir Street-Dokki., 12311 Cairo., Egypt.

We study the magnetoresistance of thin films of the ferromagnetic Heusler compounds Cu_2MnAl and Co_2MnSi. The Heusler thin films are prepared by UHV magnetron sputtering and shaped into rectangular bars with a width between 1 μm and 50 μm by optical lithography. The magnetoresistance is measured in magnetic fields up to 4 T and for the orientation of the field parallel and perpendicular to the in-

plane current. In the as-prepared state the Heusler alloy films are non-ferromagnetic and exhibit a very small magnetoresisitance only. The magnetoresistance strongly increases when the ferromagnetism gradually develops after step by step thermal annealing at high temperatures and decreases again when the magnetic moment approaches its maximum value. The magnetoresistance is dominated by an isotropic spin disorder contribution; only in the state with the maximum magnetic moment an additional small anisotropic magnetoresistance (AMR) can be resolved.

KR 10.74 Tue 10:45 Poster A

Large photoconductivity of $La_{0.7}Ca_{0.3}MnO_{3-\delta}/SrTiO_3$ heterostructures — •Elke Beyreuther[1], Andreas Thiessen[1], Stefan Grafström[1], Kathrin Dörr[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden — [2]Institut für Metallische Werkstoffe, IFW Dresden, D-01171 Dresden

The electric resistivity of stoichiometric and oxygen-deficient epitaxial 10-nm-thick $La_{0.7}Ca_{0.3}MnO_3$ thin films on $SrTiO_3$ under photoexcitation has been investigated systematically. In contrast to the as-prepared film, the oxygen-deficient one exhibits a pronounced photoinduced decrease of the resistivity of up to five orders of magnitude at low temperatures.

A detailed analysis of the resistivity as a function of illumination intensity and wavelength (visible to ultraviolet range) is presented for the bare substrate as well as for the film/substrate heterostructure. The roles of carrier generation in the film and carrier injection from the substrate, which both contribute to the observed effects, are discussed.

KR 10.75 Tue 10:45 Poster A

X-Ray magnetic circular dichroism (XMCD) study of magnetite (Fe_3O_4) thin films on semiconducting substrates — •Dominik Kufer, Markus Paul, Andreas Müller, Christian Praetorius, Annemarie Köhl, Kai Fauth, Michael Sing, and Ralph Claessen — Lehrstuhl für Experimentelle Physik 4, Universität Würzburg, Germany

Thin films of magnetite have attracted enormous research interest in recent years because of their electronic and magnetic properties. Bulk magnetite shows ferrimagnetic ordering with a theoretically predicted magnetic moment of $4\mu_B$ per formula unit below a favorably high Curie temperature of 850 K. However, structural, electronic and magnetic properties of thin films depend on choice of substrate, deposition method, and various process parameters. We have investigated the magnetic properties of epitaxial Fe_3O_4 thin films on the technologically relevant semiconducting substrates ZnO and GaAs by means of XMCD. Thin films were deposited by oxygen-assisted MBE and characterized by LEED, XPS and XRD. XMCD measurements were performed on samples with film thicknesses ranging from 3 to 40 nm, grown both *ex situ* as well as *in situ* shortly before data acquisition in total electron yield (TEY) mode. Our XMCD results confirm rather reduced magnetic moments in comparison with Fe_3O_4 bulk values [1]. Sum rule evaluation leads to spin magnetic moments in the range of 0.7-1.0μ_B per atom and nearly vanishing orbital moments for both substrates.

[1] A.Müller *et al.*, arXiv:0911.3572

KR 10.76 Tue 10:45 Poster A

Magnetic anisotropy of Zn-substituted magnetite studied by ferromagnetic resonance — •Themistoklis Sidiropoulos, Deepak Venkateshvaran, Andreas Brandlmaier, Matthias Althammer, Matthias Opel, Rudolf Gross, and Sebastian T.B. Goennenwein — Walther-Meiner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany

Ferromagnetic resonance (FMR) is a powerful technique for the investigation of the magnetic anisotropy in ferromagnetic thin films. Here, we use FMR to study the magnetic anisotropy of $Zn_xFe_{3-x}O_4$, a derivative of Fe_3O_4. We have grown coherently strained, epitaxial $Zn_xFe_{3-x}O_4$ thin films on MgO (001) substrates using pulsed laser deposition, monitored by an in situ RHEED system. Two sets of $Zn_xFe_{3-x}O_4$ films (with x = 0, 0.1, 0.33, 0.5 and 0.9) were deposited, one in pure Ar, the other in an Ar/O_2 (99:1) mixture. X-ray diffraction measurements indicate high crystallinity, as evident from a FWHM of 0.04° in the rocking curves for the $Zn_xFe_{3-x}O_4$ (004) reflection. Previously, we demonstrated that $Zn_xFe_{3-x}O_4$ shows an appreciable tunability in both its magnetic and transport properties, depending on the Zn concentration and the growth atmosphere [1]. In this study, we discuss the evolution of the magnetic anisotropy with Zn concentration, growth atmosphere and temperature.

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[1] D. Venkateshvaran et al., Phys. Rev. B **79**, 134405 (2009).

KR 10.77 Tue 10:45 Poster A

Field and temperature dependence of spin and heat transport in dimerized spin 1/2 chains. — •Stephan Langer[1], Fabian Heidrich-Meisner[1], Rachid Darradi[2], and Wolfram Brenig[2] — [1]Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, LMU München, Germany — [2]Institute for Theoretical Physics, Technical University of Braunschweig, Germany

We study the spin and heat conductivity of dimerized spin 1/2 chains in homogeneous magnetic fields at finite temperatures. Tuning the strength of the dimerization this model connects the limit of weakly coupled dimers to the Heisenberg chain. Our goal is to understand the dependence of heat and spin transport on the magnetic field, the temperature and the strength of dimerization. At zero temperature the model undergoes a field induced quantum phase transition from a dimerized into a Luttinger liquid phase. We search for signs of this transition in the spin and heat conductivity. Using exact diagonalization we calculate the Drude weights, the frequency dependence of the conductivities and the corresponding integrated spectral weights.

A similar transition from a gapped into a Luttinger Liquid phase is observed in spin ladder materials that have a comparably small exchange coupling, allowing experimentalists to probe transport at finite temperatures and fields. This serves as an additional motivation of our study.

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KR 10.78 Tue 10:45 Poster A

Magnetic and Structural Properties of $La_{1-x}Th_xCrO_3$ and $LaCr_{1-y}Ti_yO_3$ — •P. Reuvekamp[1], R. K. Kremer[1], and F. S. Razavi[2] — [1]Max Planck Institut fuer Festkoerperforschung, — [2]Department of Physics, Brock University, St. Catharines, Ontario, L2S 3A1, Canada

The magnetic properties of ceramic samples of $La_{1-x}Th_xCrO_3$ and $LaCr_{1-y}Ti_yO_3$ were investigated. In order to improve the chemical homogeneity and stoichiometry, the ceramic samples were prepared by the citrate-pyrolysis synthesis route. X-ray investigations of these samples revealed that all the phases maintained their orthorhombic structure, however with different mass densities. The substitution of Th for La does not have effect on the magnetic properties of $LaCrO_3$ with the Néel temperature remaining close to 290 K whereas, replacing Ti for Cr reduces the Néel temperature to a minimum of 237 K for y = 0.2.

KR 10.79 Tue 10:45 Poster A

Magneto-Optic Measurements of Magnetic Multilayers in Extreme Ultraviolet Range — •Roman Adam, Patrik Grychtol, Stefan Cramm, and Claus Schneider — Institute of Solid State Research IFF-9, Research Center Jülich, D-52425

We performed static and time-resolved magneto-optic measurements on Co/Si-wedge/Ni/Fe and NiFe/MgO/Co multilayers using resonant scattering of extreme ultraviolet (XUV) radiation tuned to the M absorption edges of cobalt (60.2 eV) and nickel (67.5 eV). By exploiting the linear magneto dichroic effect close to the Brewster angle a huge magnetic contrast of up to 80% from the top Co and 20 % from the buried NiFe layer upon magnetization reversal could be obtained. In order to map the magnitude of the dichroism, angular and energy dependent scans of the magnetic asymmetry were performed and compared with magneto-optical simulations. The magneto-optical response of a multilayer system to a magnetic pulse excitation results in element-specific oscillations in a frequency range of 3 to 6.5 GHz associated with magnetization dynamics of the individual Co and NiFe layers. Presented results demonstrate the feasibility of element-specific magneto-dynamic studies in magnetic multilayers in XUV spectral range.

KR 10.80 Tue 10:45 Poster A

Investigation of depletion state of high temperature protective coatings — •Iulian Teliban[1], Claas Thede[1], Steffen Chemnitz[1], Christoph Bechtold[1], Thomas Hüttel[2], Krasimir Aleksandrov[3], Willem Quadakkers[2], Michael Schütze[3], and

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In many industrial applications metallic and non-metallic protective coatings are applied to protect against oxidation, corrosion or physical degradation. To date, practical non-destructive methods for the measurement of the depletion state of the coating during the operation time do not exist. By integration of magnetic phases into the coating and measuring the magnitude of the magnetic properties important information about the coating's condition can be provided.

A new technique using frequency mixing is presented to investigate the thickness of the coatings based on their magnetic properties. The performance of the sensor was investigated using magnetic samples with defined properties and thicknesses ($Fe_{67}Co_{18}B_{14}Si_1$ multilayers), [1]. Common protective coatings consisting of a paramagnetic MCrAlY matrix in which the sensor phase (Cr, Fe) is embedded and new types of coatings based on $Al_{1-x}Cr_xN$ ($x = 0.02 \div 0.07$) are analyzed with the new technique in different stages of usage (oxidation).

Founding by the DFG via the SPP 1299 is gratefully acknowledged.

[1] I. Teliban, C. Thede, S. Chemnitz, C. Bechtold, W. J. Quadakkers, M. Schütze, and E. Quandt, Rev. Sci. Instrum. 80, 115106 (2009).