MA 13: Poster Ia: Electron Theory (1); Magnetic Imaging (2,3); Thin Films (4-25); MSMA (26-33); Magn. Semiconductors (34-42); Magn. Half Metals and Oxides (43-60)

Time: Tuesday 10:15–13:00 Location: P1A

MA 13.1 Tue 10:15 P1A

Exact thermodynamics of the extended Hubbard model for a cubic cluster — •David Zwicker and Rolf Schumann — Institute for Theoretical Physics, TU Dresden, Dresden D-01062, Germany

The Hubbard model extended by nearest-neighbor Coulomb and Heisenberg exchange interaction for an eight-site cubic cluster is studied by means of an exact diagonalization using all known interaction parameter-independent symmetries. The ground state plots in dependence of the model parameters for the complete parameter space show a multitude of ground state crossings for all occupation numbers. We determine the ground state phase diagram in dependence of the chemical potential μ, hence describing the cubic cluster gas. Within the standard Hubbard model, we find 2-4 and 6-8 degeneration points (DPs) for a wide parameter region, i.e. steps in $n(\mu)$ higher than one. These DPs can be destroyed by applying a magnetic field h or a very high correlation energy U. The critical field h_{crit} in dependence on U is calculated. Furthermore, the influence of the additional interactions onto the thermodynamic properties is studied.

MA 13.2 Tue 10:15 P1A

Setup of a sub-Kelvin scanning tunneling microscope — •Lei Zhang and Wulf Wulfhekel — Physikalisches Institut, Universität Karlsruhe, Wolfgang-Gaede Strasse 1, 76131 Karlsruhe, Germany

A new ultra-high vacuum sub-Kelvin scanning tunneling microscope with low noise, high stability and high energy resolution <0.1 meV was developed for the measurement of magnetic and vibronic excitations. The construction of the three stage cryostat is finished. The first stage is cooled with liquid N_2 with 10 W cooling power, the 2nd stage with liquid He^4 with 40 mW. The third stage uses a closed-cycle Joule-Thomson refrigerator (1 mW) with either He^4 or He^3 to cool down the STM to 0.92 K (He^4) and below 500 mK with He^3. The cryostat has a very low liquid helium consumption of only 50 ml per hour and standing times of up to 200 hours. The STM has been tested at room temperature in atmosphere, and the vacuum chamber for the STM and sample preparation have been built.

MA 13.3 Tue 10:15 P1A

A New UHV Operating Scanning X-Ray Microscope at BESSY, Berlin — •Markus Weigand[1], Kai Fauth[2], Eberhard Goering[1], Christian Wolter[1], Brigitte Baretzky[1], Marcel Mayer[1], Corinne Grévent[1], Rolf Follath[3], and Christian Jung[3] — [1]MPI f. Metallforschung, Stuttgart — [2]Uni Würzburg — [3]Bessy, Berlin

Based on the proven principle of the ALS STX microscope a new scanning soft x-ray microscope has been further developed in cooperation with ACCEL GmbH opening new frontiers in x-ray microscopy.

This microscope is constructed to work in transmission, total electron yield, as well as in reflection mode. In contrast to STXMs available up to now, not only the conventional helium mode, but also UHV operation is possible. In this configuration a UHV transfer and load lock system connects the SXM with a UHV sample preparation chamber.

A main focus of the instrument is static and dynamic XMCD imaging. For this purpose, several dedicated sample holders, one of them motorized rotatable, can be used together with an adjustable magnet system, allowing to apply magnetic fields of +/-0,4T in and out of plane.

The machine will be installed at a new APPLE II-type undulator beamline at BESSY. This SXM will also be available for external users. The development of Fresnel Zone Plates, for improving the lateral resolution, based on the concept of Atomic Layer Deposition, is in progress.

MA 13.4 Tue 10:15 P1A

Non-Linear Magnetic Vortex Gyration — •André Drews[1], Benjamin Krüger[2], Stellan Bohlens[2], Markus Bolte[1], and Guido Meier[1] — [1]Institut für Angewandte Physik und Zentrum für Miktrostrukturforschung, Universität Hamburg, Hamburg, Germany — [2]I. Institut für Theoretische Physik, Universität Hamburg, Hamburg, Germany

Magnetic vortices occur in disk- or square-shaped samples of a few hundred nanometers in soft magnetic materials. When applying an external current the vortex core gyrates around its equilibrium position. For small current amplitudes the trajectory of the gyration can be described analytically by a harmonic oscillator [1,2], for larger amplitudes the trajectory becomes nonlinear [3]. In this work the nonlinear motion of vortex cores in square-shaped samples is investigated. The nonlinear analytical equation of motion of the vortex core is solved numerically by a Runge-Kutta method. The analytical results match well with the results from micromagnetic simulations. The amplitude and frequency of the gyration in dependence on the excitation amplitude are investigated, and it is shown that with increasing excitation amplitude the nonlinearities and the blue shift of the resonance frequency increase. For varying lengths and thicknesses of permalloy squares the limits of linear vortex gyration are determined.

[1] B. Krüger et al., Phys. Rev. B. 76, 224426 (2007).
[2] A. Drews et al., Phys. Rev. B. 77, 094413 (2008).
[3] K.-S. Lee and S.-K. Kim, Appl. Phys. Lett. 91, 132511 (2007).

MA 13.5 Tue 10:15 P1A

Model samples for magneto-impedance measurements — •Saleh Getlawi, Markus König, Haibin Gao, Michael R. Koblischka, and Uwe Hartmann — Experimental Physics, Saarland University, Campus C 6 3, 66123 Saarbrücken, Germany

The growing interest in the magneto-impedance (MI) effect is mainly caused by the possible use of MI in high-sensitivity magnetic field detectors or magnetic recording heads. Observations of MI have been mainly confined to amorphous wires, magnetic multilayers and ribbon samples. Here, it is difficult to obtain the magnetic domain configuration. In order to find a relation between the magnetic domain structure and the size of the MI effect, we decided to perform measurements on model samples consisting of permalloy ($Ni_{81}Fe_{19}$, Py) nanowires prepared by means of electron beam lithography and lift-off process. Wires and other structures (rectangle, circles) were manufactured with different parameters (width, length, size, thickness, etc.). Py enables the magnetization switching process to be controlled artificially by engineering the sample geometry, Thus, there are manifold possibilities to create different domain patterns. For even smaller structures and to create pinning sites, small notches for domain pinning are manufactured using focused ion beam (FIB) milling, the optimum parameters of which (dose, ion current) were determined in a recent work [2]. Finally, the magnetic structure of our samples and MI effects are confirmed by magnetic force microscopy (MFM) observations and transport measurements.

[1] S. Getlawi et al., Superlattices and Microstructures 44, 699 (2008)

MA 13.6 Tue 10:15 P1A

Parallel XMCD and XRMS measurements with ALICE — •Stefan Buschhorn, Frank A. Brüssing, Denise Erb, Melanie Ewerlin, Radu Abrudan, and Hartmut Zabel — Experimentalphysik IV, Ruhr-Universität Bochum, 44780 Bochum

X-ray Magnetic Circular Dichroism (XMCD) is nowadays an established tool in thin film magnetism. The classical way to detect XMCD is by working either in transmission geometry or using Total Electron Yield (TEY) or Fluorescence Yield (FY) as a measure for absorption. These two signals provide surface sensitive and more bulk-like information on the magnetization, but no proper depth profile of the magnetisation. This problem is circumvented by measuring the X-ray Resonant Magnetic Scattering (XMRS) signal in $\Theta - 2\Theta$ geometry. A depth-resolved magnetisation profile for both single- and multilayer samples is then available by tuning the energy to the resonant edges for the respective elements. Additionally, in scattering geometry the magnetic coupling between laterally structured samples is accessible with diffuse scattering.

We present data taken with the ALICE chamber, where all three signals can be measured at once: TEY, FY and XRMS. A comparison is made between the different absorption/reflection spectra, showing the main differences between drain current, fluorescence and reflectivity measurements for a standard sample (Py) and a multilayered spinvalve system (Co/Cr/Fe/Cr).

MA 13.7 Tue 10:15 P1A

The reflectometer Super ADAM at ILL — •Max Wolff[1,2,3], Kyrill Zhernenkov[1], Andrew Wildes[2,3], Philipp Gutfreund[1,2], Jörg Meermann[1], Hakan Rundlof[3], Boris Toperverg[3], Adrian Rennie[3], Björgvin Hjörvarsson[3], and Hartmut Zabel[1] — [1]Institute for Solid State Physics/EP IV, Ruhr-University Bochum, Germany. — [2]Insitute Laue-Langevin, Grenoble, France. — [3]Materials Physics, Uppsala University, Sweden.

The angle dispersive neutron reflectometer ADAM at the ILL offers high flux combined with an excellent Q resolution and full polarization analysis with privileged access for the German and Swedisch user comunity. We will give a brief overview on the most recent improvements and most outstanding results obtained during the last years.

Presently a major update of the reflectometer to Super ADAM is in progress. It will combine two possible setups. A high resolution and a high intensity mode on the same monochromatic instrument. To account for this we will use a intercalated graphite monocromator. We expect unique possibilities for the investigation of magnetic thin films due to the high flux, the low background and excellent polarization analysis. A brief report on the status of the project will be given.

MA 13.8 Tue 10:15 P1A

In situ low temperature ac-susceptibility measurements on ion bombarded AlFe thin films — •Moritz Trautvetter, Ulf Wiedwald, and Paul Ziemann — Universität Ulm, Institut für Festkörperphysik, 89069 Ulm, Germany

In its chemically ordered state (B2) Al_xFe_{1-x} is paramagnetic at room temperature in the composition range of $30 < x < 50$ at% and can be switched to a ferromagnetic behavior by inducing chemical disorder [1]. For this purpose, ion irradiations are performed at various temperatures. In detail, thin films (ca. 60 nm) of AlFe (composition range as given above) were grown on Sapphire by Pulsed Laser Deposition at 300 K. As prepared $Al_{45}Fe_{55}$films are ferromagnetic with μ= 0,77 μ_B/per formula unit indicating a high degree of disorder. After annealing at 600°C for 2h under hydrogen atmosphere, a reduction of the magnetization to μ= 0,16 μ_B/f.u. is observed in accordance with the formation of an at least partially ordered B2 structure (bcc). The disorder due to the subsequent ion irradiation with 200 keV Ar^+ ions leads to an enhancement of the AlFe magnetization. This effect is studied in situ as a function of ion fluence and temperature by means of low temperature ac-susceptometry.

[1] P. Shukla, M.Wortis, Phys Rev B 21, 159 (1980)

MA 13.9 Tue 10:15 P1A

Growth of epitaxial $CaRuO_3$ films — •Markus Wissinger[1,2], Dirk Fuchs[1], Rainer Fromknecht[1], Rudolf Schneider[1], and Hilbert v.Löhneysen[1,2] — [1]Institut für Festkörperphysik, Forschungszentrum Karlsruhe, Postfach 3640, 76021 Karlsruhe, Germany — [2]Universität Karlsruhe, 76128 Karlsruhe, Germany

In this work we report on the growth of $CaRuO_3$ films by the pulsed laser deposition (PLD) technique. The films were deposited from stoichiometric targets which were produced by standard solid state reaction. Powder X-ray diffraction (XRD) demonstrated the impurity free orthorhombic Pbnm structure of the targets. The films were grown on (001) oriented $(LaAlO_3)_{0.3}(SrAl_{0.5}Ta_{0.5}O_3)_{0.7}$ and (110) $NdGaO_3$ single crystal substrates. The growth mode and film thickness were studied by in-situ reflection high energy electron diffraction. The composition of the films was checked by electron dispersive x-ray analysis and Rutherford backscattering spectrometry. The substrate temperature, Ts, the oxygen partial pressure, P(O2), and the target-substrate distance, d, were optimized with respect to the crystallinity of the films. The mosaic spread of the films and the of-plane lattice constant were determined from rocking curves and $\theta/2\theta$ scans on 00l reflections, respectively.

MA 13.10 Tue 10:15 P1A

crystallographic structure and magnetic properties of electrodeposited Co- rich Co-Pt films — •manvendra khatri[1,2], heike schlörb[1], ludwig schultz[1,2], and sebastian fähler[1,2] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box 27 00 16, D-01171 Dresden, Germany — [2]Institute for Solid State Physics, Department of Physics, Dresden University of Technology, 01062 Dresden, Germany

Co- rich Co-Pt alloy films have been grown by electrodeposition on Au seed layers. The influence of deposition current density on chemical composition, structure, microstructure and magnetic properties of the films has been investigated. Due to the superposition of the fcc Co-Pt (111) and hcp Co-Pt (002) planes the information supplied by XRD in conventional Bragg Brentano geometry was of limited value. Hence detailed texture measurements have been performed in order to understand the dependence of magnetic properties on phase composition and texture perfection. By comparing the integrated intensity ratio of fcc (200) to hcp (002) and fcc (111) reflections taken from pole figure measurements, it is possible to estimate the formation of hcp phase in the films with respect to current density. The integrated intensity ratio decreases with current density, which indicates the increase in the (002) texture of hcp in the film. The presence of (002) pole of hcp at higher current density indicates the textured growth of the film with c-axis out of plane. The decrease in the integrated intensity ratio is accompanied by an improvement of the out-of plane magnetic properties.

MA 13.11 Tue 10:15 P1A

Epitaxial $RECo_5$ single layer and bilayer films — •Marietta Seifert, Felix Fleischhauer, Ajit Patra, Volker Neu, and Ludwig Schultz — IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany

Intermetallic RECo phases are widely used in permanent magnet applications due to their large magnetocrystalline anisotropy. Therefore in previous work we developed epitaxial growth of thin $SmCo_5$ and $PrCo_7$ films on Cr buffered MgO(110) substrates with high coercivity or energy density [1,2]. $RECo_5$ phases with RE = Pr or Nd are also known to exhibit spin reorientation transition from an uniaxial state into easy-cone or easy-plane arrangement and are thus interesting from a fundamental point of view.

In this work we present the temperature and field dependent magnetic behaviour of epitaxial $NdCo_5$, $SmCo_5$ and $PrCo_5$ single layer films and bilayers. Epitaxial $NdCo_5$ films grow with the same single orientation of the *c*-axis established for $SmCo_5$ and exhibit an easy-axis to easy-plane transition. Bilayers of $PrCo_5$ and $SmCo_5$ likewise grow epitaxially with one common orientation of the *c*-axis throughout the layer stack. Despite their largely different coercivity when grown as single layers the bilayer films reverse magnetization in one large irreversible step indicating a strong interlayer exchange coupling.

[1] A. Singh, V. Neu, R. Tamm, K. Rao, S. Fähler, W. Skrotzki, L. Schultz, B. Holzapfel, JAP **99** 08E917 (2006)

[2] A. Patra, V. Neu, S. Fähler, L. Schultz, J. Phys. D: Appl. Phys. **40** (2007) 7261-7266

MA 13.12 Tue 10:15 P1A

Epitaxial Fe_3Si films: Structure, electrical and magnetic properties — •Joachim Schumann[1], Hartmut Vinzelberg[1], Christoph Deneke[1], Dieter Elefant[1], Jürgen Thomas[1], Ernest Arushanov[1,2], and Oliver G. Schmidt[1] — [1]IFW Dresden, P.O.Box 270116, D-01171 Dresden, Germany — [2]Institute of Applied Physics, 277028 Chisinau, Moldowa

Epitaxial Fe_3Si films have been prepared by means of UHV electron beam co-evaporation on GaAs (100) substrates for studies on planar [1] and cylindrically shaped [2] samples. High resolution TEM shows that the films are grown with a high crystalline quality and a good interface perfection what makes them comparable with the best Fe_3Si MBE layers. The electrical measurements present a low-temperature T^3 term describing the anomalous single-magnon scattering processes in half-metallic materials. So, the hypothesis of half-metallic ferromagnetism in Fe_3Si can be considered as confirmed [1]. The films have an anisotropic magnetoresistance in low magnetic fields. In high magnetic fields a negative longitudinal and transverse magnetoresistance (MR) was found. In the vicinity of 200 K the MR shows a maximum of about 1.5% at fields of about 8 T. The magnetic moment was determined as 0.86 μ_B/atom close to the bulk value of Fe_3Si.

[1] H. Vinzelberg et al., J. Appl. Phys. **104**, 093707 (2008).
[2] C. Deneke, et al., phys.stat.sol.(c) **5**, 2704 (2008).

MA 13.13 Tue 10:15 P1A

Sputtering deposition of epitaxial $Co_2Mn_{1-x}Fe_xSi$ and Co_2MnAl films — •Enrique Vilanova Vidal, Horst Schneider, and Gerhard Jakob — Institut für Physik, Johannes Gutenberg-Universität Mainz

Recently it has been discussed whether the Heusler compounds $Co_2Mn_{0.5}Fe_{0.5}Si$ and Co_2MnAl are halfmetallic systems. The comparison of band structure calculations with experimental results indicate that electron correlations play an important role in this question. In order to gain further insight into the electronic structure

of these materials, we have prepared thin films of $Co_2Mn_{0.5}Fe_{0.5}Si$ and Co_2MnAl. These films were grown by cathode sputtering on MgO (100) with and without MgO buffer layer using an UHV deposition system. The investigated films grow epitaxially and possess the fully ordered $L2_1$ Heusler structure. We discuss the deposition procedure and measurements of composition, crystal structure and magnetic properties of the films with respect to the electronic structure of the alloys.

MA 13.14 Tue 10:15 P1A

Fe monolayers on InAs(001): An in situ study of surface, interface and volume magnetic anisotropy — •Florian M. Römer, Christoph Hassel, Khalil Zakeri, Cihan Tomaz, Igor Barsukov, Ralf Meckenstock, Jürgen Lindner, and Michael Farle — Fachbereich Physik and Center for Nanointegration (CeNIDE), Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany.

The magnetic anisotropy of epitaxial Fe films with thicknesses in the range of $2-142$ monolayers (ML) grown on $\{4\times 2\}$ reconstructed InAs(001) was investigated by *in situ* ferromagnetic resonance. The easy magnetization direction was found to be parallel to the $[1\bar{1}0]$-direction for Fe films below 4 monolayers, while it rotates by 45° toward the [100]-direction. It is observed that both surface-interface and volume contribution to the perpendicular anisotropy favor an easy axis perpendicular to the film plane. The cubic surface-interface anisotropy is relatively large with easy axes along $\langle 1\bar{1}0\rangle$-directions in contrast to the volume contribution which favors easy axes along the $\langle 110\rangle$-directions. The volume contribution is found to be larger than the Fe bulk cubic anisotropy. A thickness independent uniaxial anisotropy has been found in films with a thickness of 2 up to 142 monolayers. Changes due to capping with Pt/Ag will be shown.

MA 13.15 Tue 10:15 P1A

Magnetooptical properties(MOKE) of spin valves based on Co, Cu or Au — Iryna Cheshko[1], •Dmytro Kutnyakhov[2], Larisa Odnodvorets[1], Sergej Protsenko[1], Sergej Nepijko[2], and Gerd Schoenhense[2] — [1]Sumy State University, 2, R.-Korsakov street, 40007, Sumy, Ukraine — [2]Institute of Physics of University Mainz, 7, Staudingerweg, 55099, Mainz, Germany

Starting from the structural and phase states of the film systems on the basis of Co, Cu and Au, we fabricated a spin valve structure as multilayer film system of Au(3)/Co(3)/Au(Cu)(6)/Co(20)/Au(40)/Cr(3)/s (s-substrate, thickness of layers in nm). The layer Co(3) is more sensible to an external magnetic field and begins the process of remagnetization of the domain structure at lower field amplitudes.

The GMR effect shows up as a variation of the resistivity as function of the magnetic field. It reflects the different fields for the remagnetization of overlayer and underlayer. Thus at the change of the external magnetic field this system is creating a bipolar electric signal with high amplitude. The layers Cr(3) and Au(40) support high adhesion to the sital(glass-ceramic) substrate and provide the electric contacts. X-ray diffraction revealed that at annealing the spin valve structures to 700 K granular solid solutions (Au, Co) or (Cu, Co) occurred. Research of magnetoresistance and magnetooptical Kerr effect (MOKE) confirmed the conclusion about the formation of granular solid solutions.

This work is collaboration between the Institute of Physics of University Mainz (Germany) and Sumy State University (Ukraine).

MA 13.16 Tue 10:15 P1A

Magnetic and structural properties of epitaxial thin films of the Heusler compounds Cu_2MnAl and Co_2MnGe — •Denise Erb, Jörg Dudek, Frank Brüssing, Gregor Nowak, Kurt Westerholt, and Hartmut Zabel — Ruhr-Universität Bochum Experimentalphysik IV / Festkörperphysik, Bochum, Deutschland

Several Heusler compounds possess half metallic properties in the ordered $L2_1$ structure, which make them promising candidates for spintronic applications. We have grown thin films of the Heusler phases Co_2MnGe and Cu_2MnAl using ion beam sputtering and UHV magnetron sputtering on MgO(100) and sapphire a-plane substrates. The structural properties were studied by x-ray diffraction and x-ray reflectivity. Epitaxial thin films with smooth surfaces can be prepared with the substrates at room temperature. The Co_2MnGe film prepared on Al_2O_3 a-plane and a 2nm V seed layer exhibits 12 well defined peaks in the in-plane rocking scan of the (022)-Bragg reflection, indicative of the growth of 3 different crystalline domains rotated by 30° relative to each other. The Heusler phase Cu_2MnAl is actually not half metallic, but exhibits model type behaviour concerning the relations between the structural and magnetic properties. It can be grown on MgO(001) with the in-plane [100]-direction rotated by 45° from the MgO [100]-direction. In the as-grown state the Cu_2MnAl film is non magnetic, ferromagnetic order starts developing when annealing above 280°C. The increasing ferromagnetic magnetization is accompanied by an increasing intensity of the (002) superstructure Bragg reflection.
The authors thank the DFG for financial support within the SFB 491.

MA 13.17 Tue 10:15 P1A

Fe- Pd thin films: A prototype system for exchange coupling? — •Thomas Schied[1,2], Jörg Buschbeck[1], Ludwig Schultz[1,2], and Sebastian Fähler[1,2] — [1]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [2]Institute for Solid State Physics, Department of Physics, Dresden University of Technology, 01062 Dresden, Germany

High performance hard magnetic films are a key requirement for applications in Micro Electro Mechanical Systems (MEMS) and as perpendicular magnetic recording media. Both applications are expected to benefit from exchange coupled hard/soft magnets. Whereas several L10 ordered systems such as Fe-Pt, Co-Pt and Fe-Pd are known to exhibit a sufficiently high magneto crystalline anisotropy, the Fe-Pd system is the only L10 system thermodynamically demixing into a high Ku hard magnetic and a high Js soft magnetic phase. In this work composition spreads of Fe-Pd are prepared by magnetron sputtering from elemental Fe and Pd targets, covering most of the composition range from the high Js Fe-rich phase to the high Ku L10 phase. Local magnetic properties are analyzed using a scanning magnetometer based on the polar magneto optical Kerr-effect. Together with structural investigations by XRD and surface morphology by AFM the key properties are analyzed locally. These information*s are used to correlate magnetic properties with composition, phase formation and micro structure. In order to obtain an alignment of the easy axis perpendicular to the substrate the influence of two different heated substrates - Si/SiO wafers without buffer and Si/SiO wafers with MgO buffer - is investigated.

MA 13.18 Tue 10:15 P1A

Electronic and magnetic properties of ferromagnetic Mn_5Ge_3(0001) epilayer on Ge(111) — •Yuriy Dedkov[1], Matthias Holder[2], Gillian Mayer[3], Mikhail Fonin[3], and Alexej Preobrajenski[4] — [1]FHI Berlin — [2]TU Dresden — [3]Uni Konstanz — [4]MAX-lab, Lund

The dramatic situation in the semiconductor spintronic can be improved by the preparation of epitaxial ferromagnetic compounds on the basis of 3*d* metals and silicon or germanium grown on the corresponding semiconducting substrates. The Mn-based materials are most promising candidates because the Curie temperature of corresponding silicides or germanides can reach room temperature. Here we present a study of the electronic structure of high-quality well-characterized epitaxial ferromagnetic Mn_5Ge_3(0001) films on Ge(111) by means of x-ray absorption spectroscopy, x-ray photoelectron spectroscopy, and spin-resolved photoelectron spectroscopy. Spin-polarization value of about +15% is measured with 21.2 eV photon energy at the Fermi level at 190 K. The experimental photoemission data is explained on the basis of available band structure calculations of ferromagnetic bulk Mn_5Ge_3.

MA 13.19 Tue 10:15 P1A

Metamagnetic domains in [Co/Pt]/Ru multilayers — •N. S. Kiselev[1,2], C. Bran[1], U. Wolff[1], L. Schultz[1], A.N. Bogdanov[1], O. Hellwig[3], V. Neu[1], and U. K. Rössler[1] — [1]IFW Dresden — [2]Donetsk Inst. for Physics & Technology — [3]Hitachi GST, San Jose

In antiferromagnetically coupled superlattices with perpendicular anisotropy, a magnetic field induces a cascade of reorientation transitions accompanied by *metamagnetic* multidomain states [1,2]. For a micromagnetic model, we derive equilibrium sizes of stripe and bubble metamagnetic domains as functions of the antiferromagnetic exchange, magnetic field, and geometrical parameters of the multilayers. Magnetic phase diagrams display three different types of metamagnetic domains which separate the ferrimagnetic state from the antiferromagnetic and the saturated ferromagnetic state, and from ferrostripe phases. Experimental investigations have been carried out for an antiferromagnetically coupled $[(Co/Pt)_8Co/Ru]_{18}$ superlattice. Magnetic force microscopy (MFM) imaging in a magnetic fields reveals peculiarities of the nucleation and evolution of metamagnetic domains. Theoretical analysis of MFM data and the magnetization curves gives a consistent description of the magnetization processes in [Co/Pt]/Ru multilayers. Demagnetization processes starting from the multidomain

metamagnetic states lead to specific remanents states, namely metamagnetic band and bubble topological defects[2].

[1] O. Hellwig, A. Berger, J. B. Kortright, E. E. Fullerton, J. Magn. Magn. Mater. **319** 13 (2007). [2] N.S. Kiselev, U. K. Rößler, A. N. Bogdanov, O. Hellwig, Appl. Phys. Lett. **93** 132507 (2008).

MA 13.20 Tue 10:15 P1A

Micromagnetic analysis of magnetic nanosystems with competing anisotropies — •Andrei A. Leonov[1,2], Ulrich K. Rössler[1], and Alexei N. Bogdanov[1] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Donetsk Institute for Physics and Technology, 83114 Donetsk, Ukraine

The interplay between cubic and uniaxial magnetic anisotropies strongly influences magnetization processes in such novel classes of nanomagnetic systems as ferromagnet-antiferromagnet bilayers, thin epilayers of diluted magnetic semiconductors, Heusler alloys, magnetic nanowires or nanoparticles.We have extended and generalized a micromagnetic model to describe magnetization processes in systems with competing magnetic anisotropies and adopted them to investigate nanomagnetic systems (see [1] and bibliography in [1]). In this contribution we apply the results of [1] for detailed analysis of recent experimental results: (i) remarkable transformation of metastable magnetic states, reorientation effects, and magnetization reversal observed in Fe-Cu-B nanoparticles [2], in (Ga,Mn)As epilayers [3], and in magnetite [4] films. (ii) magnetic-field-driven evolution of magnetic domain walls in nanoconstrictions [5]. (iii) calculation of the parameters for multidomain patterns in (Ga,Mn)As films with perpendicular anisotropy [1].

[1] A.A.Leonov et al. J. Appl. Phys. **104**, 084304 (2008). [2] N. Duxin et al., Langmuir **16**, 11 (2000). [3] K.Pappert et al., Appl. Phys. Lett. **90**, 062109 (2007). [4] A. Brandlmaier et al., Phys. Rev. B **77**, 104445 (2008). [5] M. Yamanouchi et al., Nature (London) **428**, 539 (2004).

MA 13.21 Tue 10:15 P1A

Coercivity analysis in highly anisotropic $PrCo_7$ films — •Volker Neu[1], Ajit Kumar Patra[1], Stephen Collocott[2], Sebastian Fähler[1], and Ludwig Schultz[1] — [1]IFW Dresden, Institute for Metallic Materials, PO Box 270116, D-01171 Dresden, Germany — [2]CSIRO Materials Science and Engineering, PO Box 218, Lindfield NSW 2070, Australia

In order to tailor the response of a magnetic material to an external magnetic field a sound understanding of the underlying magnetization process is required. For permanent magnet materials this central question culminates in understanding the origin of coercivity. The known concepts of coercivity analysis, the micromagnetic model and the global or phenomenological model are applied to a permanent magnet film based on epitaxial $PrCo_7$. Such films possess a single orientation of the crystallographic c-axis within the film plane and a square shaped hysteresis with large coercivity. The temperature dependent coercivity is compared on one hand with the expected nucleation or depinning field based on the independently determined anisotropy constants and on the other hand is expressed as a thermally activated domain wall movement within a certain activation volume. For this, the fluctuation field as a function of temperature is extracted from magnetization relaxation and irreversible susceptibility measurements. A consistent description of the data is possible under the assumption of weak pinning. The analysis is however complicated by the spin reorientation from uniaxial anisotropy at high temperature to an easy-cone anisotropy below 110K.

MA 13.22 Tue 10:15 P1A

Electronic structure of a stabilized bulk-like α-Mn thick film on W(110) — •Elena Voloshina[1], Yuriy Dedkov[2], and Manuel Richter[3] — [1]Institut für Chemie und Biochemie - Physikalische und Theoretische Chemie, Freie Universität Berlin, Germany — [2]Fritz-Haber Institut, Berlin, Germany — [3]IFW Dresden, P. O. Box 270 116, 01171 Dresden, Germany

We report on the successful stabilization of thick bulk-like α-Mn films with (110) orientation on W(110) substrate. The observed (3×3) patterns are consistent with the presented growth model. Angle-resolved photoemission spectra show weak dispersions of the valence band electronic states. These PE data are analyzed on the basis of DFT calculations for non-magnetic bcc α-Mn. The observed weak dispersions are caused by the large number of inequivalent Mn atoms of the α-Mn structure.

MA 13.23 Tue 10:15 P1A

Magneto-elastic coupling in $LaCoO_3$ thin films — •Erhan Arac[1,2], Dirk Fuchs[1], Fadi El-Hallak[3], Rudolf Schneider[1], and Hilbert von Löhneysen[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [2]Physikalisches Institut, Universität Karlsruhe, 76128 Karlsruhe, Germany — [3]1. Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, German

The magnetization of epitaxial $LaCoO_3$ thin films with respect to magnitude and orientation of the strain is investigated. The magnitude of the epitaxial tensile strain is varied by the growth of thin films on (001) oriented $SrLaAlO_4$, $SrLaGa_4$, $(LaAlO_3)_0.3(Sr_2AlTaO_6)_0.7$ (LSAT) and $SrTiO_3$ single crystal substrates while the orientation is changed by the growth on (001),(110) and (111) oriented LSAT substrates by pulsed laser deposition (PLD). The magneto-elastic constant B_1 is determined by "area method". The negative sign implies that in-plane magnetization is favoured which is convenient with obtained in-plane hysteresis loops of (001) samples. Moreover, magnetic anisotropy measurements of (001) and (110) samples revealed 4-fold and 2-fold symmetry. The uniaxial magnetic anisotropy in (110) film can be explained by the dominance of the stress anisotropy over magneto-crystalline anisotropy effects.

MA 13.24 Tue 10:15 P1A

Geometry and magnetic structure of uranium along the tetragonal epitaxial Bain path — •Stephan Schönecker, Manuel Richter, Klaus Koepernik, and Helmut Eschrig — IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany

Epitaxially manufactured structures grown pseudomorphically on suitable substrates provide a way to stabilise non-equilibrium structures of materials. This includes grown films which posses a large lattice misfit between substrate and film material under equilibrium conditions, but also if the structure grown differs from the equilibrium structure of the bulk film material. Large misfits do not necessarily mean large lateral stress. Theory can help to predict e.g. geometry, stresses and magnetic properties of pseudomorphically grown metal films. In this work, we considered the epitaxial Bain path (e.g. [1]) of elemental uranium, which provides a reasonable description of tetragonally distorted films on substrates. We employed density functional calculation in the implementation of the full potential local orbital program package FPLO [2]. We found three meta-stable tetragonal phases, in addition a ferromagnetic state close to the fcc phase.

[1] P. M. Marcus, F. Jona, and S. L. Qiu, Phys. Rev. B **66**, 064111 (2002)
[2] K. Koepernik and H. Eschrig, Phys. Rev. B **59**, 1743 (1999); http://www.fplo.de

MA 13.25 Tue 10:15 P1A

The strained epitaxial Nd-Fe-B films by mechanical elongation — •Ah-Ram Kwon[1], Volker Neu[1], Vlakimir Matias[2], Jens Hänisch[1,2], Ruben Hühne[1], Bernhard Holzapfel[1], Ludwig Schultz[1], and Sebastian Fähler[1] — [1]IFW Dresden, P.O. Box 270116 D-01171 Dresden — [2]Los Alamos National Laboratory, Mail Stop T004, Los Alamos NM 8545 USA

Though it is well known that a variation of lattice constants strongly influences the functional properties of materials, most of the experiments are limited to hydrostatic pressure or biaxial stress. Here we present an approach, which impresses a large uniaxial strain on epitaxially grown films in order to tune their functional properties. A ductile Hastelloy substrate covered with a (001) oriented ion beam assisted MgO layer is used. Conventional mechanical elongation after deposition breaks the symmetry within the substrate plane compared to the as-deposited state. Consequences are exemplarily examined for an epitaxial hard magnetic Nd2Fe14B film strained by 2%. Though magnetostriction is usually considered to be negligible in this material exhibiting a high magnetocrystalline anisotropy, the uniaxial strain results in an elliptical distortion of the in-plane anisotropy below the spin-reorientation temperature. Our approach is versatile to study the influence of large strain on various materials, as the used MgO (001) layer is a common substrate for epitaxial growth.

MA 13.26 Tue 10:15 P1A

Thin film growth and shape memory in the Heusler compound Mn2NiGa — •Catherine Jenkins[1,2], Tobias Eichhorn[2], Ramamoorthy Ramesh[1], and Gerhard Jakob[2] — [1]UC Berkeley, Berkeley, 94720, USA — [2]University Mainz, 55122 Mainz, Germany

The ferromagnetic shape memory effect has been known for more than a decade in cubic to tetragonal Ni2MnGa with a maximum of 10% strain in single crystals. Recent work in fully epitaxial single crystals of Ni2MnGa on MgO and Al2O3 demonstrated our group*s ability to process high quality ferromagnetic shape memory films in novel form [1]. Mn2NiGa has a higher Curie temperature in the stoichiometric compound and an analogous crystal structure to the prototypical Ni2MnGa but due to the higher tetragonal distortion with transformation the theoretical strain is closer to 20%. The first thin films of these compounds are synthesized and the shape memory effect is investigated. Comparison in the magnetic data is made to calculations.

[1] Jenkins et al, APL, December 2008. [2] Liu et al, Phys. Rev. B, 74, 054435 (2006) [3] Barman and Chakrabarti, PRB April 2008.

MA 13.27 Tue 10:15 P1A

Sputter deposited epitaxial Ni-Mn-Ga films on various substrates — •Anja Backen[1,2], Stefan Kaufmann[1], Jörg Buschbeck[1,2], Ludwig Schultz[1,2], and Sebastian Fähler[1] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box: 270116, 01171 Dresden, Germany — [2]Departement of Mechanical Engineering, Institute for Material Science, Dresden University of Technology, 01062 Dresden, Germany

Due to their large strain up to 10 % magnetic shape memory alloys (MSM) are a promising class of active materials that can be integrated in microdevices. The deposition of epitaxial films is most suitable for this application since significant strains have only been observed in bulk single crystals. Tailoring the microstructure of the films is crucial in order to obtain high strains by magnetically induced reorientation (MIR) via twin boundary motion. Extensive research effort has been put into the investigation of the MSM alloy Ni-Mn-Ga which was deposited on various substrates (Al_2O_3, $SrTiO_3$, NaCl, MgO) by DC sputtering. In order to release the films from the substrates the concept of a sacrificial buffer layer is used. We focus on epitaxial Ni-Mn-Ga films deposited on MgO substrates with Cr buffers while varying the deposition parameters. First results on both constraint and freestanding films will be presented.

MA 13.28 Tue 10:15 P1A

Composition and microstructure of sputtered Ni-Mn-Ga magnetic shape memory thin films — •J. Petersen, Y. Luo, S. G. Mayr, and K. Samwer — I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Ni-Mn-Ga films close to the composition of $Ni_{50}Mn_{30}Ga_{20}$ were sputter deposited onto different substrates, e.g. thermally oxidized silicon and NaCl(100). Object to the investigation is the influence of deposition parameters on the resulting film composition, phase and microstructure. The Ni content of the original sputtering target ($Ni_{50}Mn_{30}Ga_{20}$) was increased to obtain a higher martensitic transformation temperature T_M above room temperature (here $T_M > 150°C$ measured by temperature dependent x-ray diffraction). First results show a significant depletion of Mn in the films with increasing deposition temperature whereas the ratio of Ni to Ga remains nearly constant. While thermally annealed films deposited at room temperature show the same 7M modulated martensitic phase and depletion of Mn, the advantage is that loss of Mn can be limited by using short annealing times and surface roughness is dramatically reduced. We acknowledge support by the BMBF - project 13N10061 MSM-sens.

MA 13.29 Tue 10:15 P1A

In-situ studies of the martensitic transformation in epitaxial Ni-Mn-Ga films — •Robert Niemann[1,2], Jörg Buschbeck[1], Oleg Heczko[1,3], Michael Thomas[1], Ludwig Schultz[1,2], and Sebastian Fähler[1,2] — [1]IFW Dresden, P.O. Box: 270116, 01171 Dresden, Germany — [2]Institute for Solid State Physics, Department of Physics, Dresden University of Technology, 01062 Dresden, Germany — [3]Institute of Physics, Academy of Science of Czech Republic, Na Slovance 2, 18205 Prague, Czech Republic

The martensitic transformation of epitaxial Ni-Mn-Ga films on rigid substrates is examined with respect to changes of structure, microstructure, magnetic and electronic properties. For this, temperature dependent atomic force microscopy (AFM), X-ray, magnetization and resistivity measurements are used. The combination of these in-situ methods give a comprehensive understanding of the martensitic transformation and allows to identify differences of constrained epitaxial films compared to bulk. Experiments show the formation of a twinned, orthorhombic martensite with high uniaxial magnetocrystalline anisotropy from the austenite around room temperature. While most features are similar to a first order transformation, the transformation proceeds continuously to lower temperatures, an effect which could be explained by the constrain of the rigid substrate. The high-resolution AFM micrographs directly reveal how martensite variants grow and show the converging of variants from different nucleation origins. A crystallographic modell is presented which explains the regular, triangular morphology observed by AFM in the martensite state.

MA 13.30 Tue 10:15 P1A

Structure and magnetism of Fe-Pd bulk alloys and nanoparticles from first principles — •Markus Ernst Gruner — Department of Physics and Center for Nanointegration CENIDE, University of Duisburg-Essen, 47048 Duisburg, Germany

In disordered off-stoichiometric $Fe_{70}Pd_{30}$ and in Fe_3Pt as well as in Ni-Mn-Ga full Heusler alloys the magnetic shape memory (MSM) effect is observed, allowing macroscopic strains of several percent to be achieved in realistic magnetic fields which opens up technological applications as nano- or microscale actuators. The underlying mechanism requires a considerable magnetocrystalline anisotropy in connection with an extremely high mobility of martensitic twin boundaries. In addition, Fe-Pt and Fe-Pd exhibit in their stoichiometric $L1_0$ phases a magnetocrystalline anisotropy energy being sufficient to entitle them for recording media applications.

This contribution presents ab initio calculations within the framework of density functional theory of the stoichiometric ordered phases of Fe-Pd as well as for disordered systems with MSM relevant composition which are covered within a supercell approach. The investigation covers bulk systems and nanometer-sized clusters which give an account on the influence of surfaces and the possible importance of multiply twinned morphologies.

This work is supported by the Deutsche Forschungsgemeinschaft through SPP 1239 and SFB 445. Part of the computations were carried out on the supercomputers of the John von Neumann Institute for Computing at Forschungszentrum Jülich.

MA 13.31 Tue 10:15 P1A

Domain models for ferromagnetic shape-memory alloys: magnetic phase diagrams, transformation and magnetization processes — •Aristide T. Onisan, Alexei N. Bogdanov, and Ulrich K. Rössler — IFW Dresden, POB 270116, 01171 Dresden

A phenomenological domain theory for magnetic shape memory materials is developed for the case of a ferromagnetic martensite with tetragonal twin variants, as a simplified approach to the archetypical Ni_2MnGa Heusler alloys. A three dimensional model is analysed that is derived from a micromagnetic continuum approach combined with piecewise linear crystal elasticity of the twin variants. The tetragonal variants are assumed to own easy-axis magnetic anisotropy. The phase theory approximation is used to treat the equilibrium domain structure which is composed of six phases describing the two magnetic domains within each of the three possible twin variants created in an austenitic cubic single crystal. Phase diagrams under magnetic fields and stresses have been calculated in the three-dimensional case for a macroscopic sample with ellipsoidal shape. We have also calculated switching fields and the theoretical maximum hysteresis for two-dimensional geometries where only two twin-variants are present and twin-rearrangement is impeded by coercivity. Our results for realistic materials parameters are compared with existing experimental data.

MA 13.32 Tue 10:15 P1A

Fe-Pd magnetic shape memory foils and films: a comparison of structural, magnetic and electronic properties — •Iris Kock, Tobias Edler, Lisa Kühnemund, and Stefan Georg Mayr — I. Physikalisches Institut, Georg-August-Universität Göttingen

Miniaturization of shape memory devices is an important challenge for application in microactuation. To ensure adequate functionality, a profound knowledge about size dependent limitations and a detailed understanding of the underlying physics is desirable. For this purpose, Fe-Pd splats (with a thickness of 60μm) that are martensitic at room temperature, were compared to vapor deposited thin films (thickness $< 1\mu$m) that were optimized by various techniques during and after growth. Especially comparison of structural, magnetic and electronic properties gives insight into substrate and surface induced constraints as well as other impacts of miniaturization. *Funded by the DFG-SPP 1239 (C4)*

MA 13.33 Tue 10:15 P1A

Influence of Surface Condition and Training on the Twin-

ning Stress of Ni-Mn-Ga Magnetic Shape-Memory Alloys — •Markus Chmielus[1,2], Katharian Rolfs[1], Cassie Witherspoon[2], Walter Reimers[3], Peter Müllner[2], and Rainer Schneider[1] — [1]SF1, Helmholtz Centre Berlin for Materials and Energy, 14109 Berlin, Germany — [2]Department of Materials Science and Engineering, Boise State University, Boise, Idaho 83725, USA — [3]Institut für Werkstoffwissenschaften und -technologien, Technische Universität Berlin, 10587 Berlin, Germany

While the effects of composition of Ni-Mn-Ga magnetic shape memory alloys (MSMAs) on structure, thermal, and magnetic properties have been well studied, effects related to the processing of MSMA single crystals have attracted less attention. Annealing, cutting, and surface preparation are known to impact the magneto-mechanical properties but no quantitative data is available. In this work, the influence of the surface roughness on the twinning stress is evaluated. During spark erosion cutting - commonly used to prepare single crystalline samples - a rough surface layer is produced. Directly after cutting, the single crystals exhibit a high twinning stress. After removal of a surface layer through electro polishing, the twinning stress reduces significantly. It is shown here, however, that a reduction of the twinning stress after each of several electro polishing steps is induced by mechanical training. This softening also occurs for unpolished Ni-Mn-Ga single crystals when subjected to the same training procedure. The results are discussed in terms of twin-surface and twin-twin interactions.

MA 13.34 Tue 10:15 P1A

Temperature dependent domain wall dynamics in compressively strained GaMnAs — •Jan Honolka[1], Liza Herrera Diez[1], Reinhard Kremer[1], Ernesto Placidi[2], Fabrizio Arciprete[2], and Klaus Kern[1] — [1]MPI für Festkörperforschung, Stuttgart — [2]Dipartimento di Fisica, Universita di Roma 'Tor Vergata'

The correlation between carrier density and magnetic properties like Tc [1] or the magnetic anisotropy [2] in GaMnAs enables the tuning of magneto-transport properties and opens new ways for magneto-logic devices[3]. A full control over magnetic reversal dynamics mediated via nucleation and propagation of domain walls (DWs) is necessary. While magneto-transport measurements only give spatially averaged information about DW dynamics we use Kerr microscopy to track individual in-plane domains in space and time. Based on the energy landscape given by the interplay of bi- and uniaxial anisotropy contributions in compressively strained GaMnAs we are able to directly observe the nucleation of DWs and their shape and mobility. At low temperatures DW nucleation and propagation depend on the crystalline directions of the film with respect to the applied magnetic field [4]. We now show the temperature dependence of the dynamics which gives valuable information for controlling DW dynamics and for the development of single DW devices.

[1] T.Dietl et al., Science 287, 1019 (2000). [2] T.Dietl, H.Ohno, and F.Matsukura, Phys. Rev. B 63, 195205 (2001). [3] D.Chiba, M.Yamanouchi, F.Matsukura, H.Ohno, Science 301, 943 (2003). [4] L. Herrera Diez et al., Phys. Rev. B 78, 155310 (2008).

MA 13.35 Tue 10:15 P1A

Effects of thermal treatment on the electronic structure of $Ga_{1-x}Mn_xAs$ — •Benjamin Schmid[1], Dominic Fertig[1], Sebastian Engelbrecht[1], Michael Sing[1], Lars Ebel[2], Charles Gould[2], Karl Brunner[2], Laurens W. Molenkamp[2], and Ralph Claessen[2] — [1]Experimentelle Physik IV, Universität Würzburg, Würzburg, Germany — [2]Experimentelle Physik III, Universität Würzburg, Würzburg, Germany

Despite intense research over the last decade the electronic structure of diluted magnetic semiconductors, especially the prototypical (Ga,Mn)As system, remains subject of controversial discussions. The interplay of substitutional and interstitial Mn and the possible exsistence of a Mn-related impurity band are two major issues. The situation is further complicated by post-growth treatments required for the improvement of the transport and magnetic properties. Photoemission spectroscopy (PES) is an outstanding tool for the investigation of electronic properties of solids, both in regard to the chemical state of ions and the conduction electrons near the Fermi-energy.
We present a detailed study of changes in the electronic structure of $Ga_{1-x}Mn_xAs$ upon various sample treatments. Effects of *ex-situ* and *in-situ* thermal treatment as well as wet-chemical etching and ion-sputtering are discussed on basis of the Mn 2*p*-doublet and the density of states in the vicinity of the Fermi-energy. The results are backed by complementary tools, i.e., low-energy electron diffraction (LEED) and atomic force/scaning tunneling microscopy (AFM/STM).

MA 13.36 Tue 10:15 P1A

Relativistic electronic structure of Mn-doped GaAs — •Ilja Turek[1], Vaclav Drchal[2], and Josef Kudrnovsky[2] — [1]Institute of Physics of Materials, ASCR, Brno, Czech Republic — [2]Institute of Physics, ASCR, Prague, Czech Republic

Electronic structure of Mn-doped GaAs diluted magnetic semiconductor is studied by means of the first-principles TB-LMTO method within the local spin-density approximation (LSDA) and the coherent potential approximation (CPA). Particular attention is paid to an interplay of chemical disorder, spin polarization and spin-orbit interaction (SOI). The results prove that the SOI has a negligible effect on integral properties (magnetic moments, densities of states) but it destroys the perfect spin polarization of states at the Fermi energy. Inspection of the Bloch spectral functions, evaluated along high-symmetry lines of the Brillouin zone, reveals that the majority spin states around the Fermi energy exhibit a very strong disorder. The minority spin states at the top of the valence band are only weakly affected by the randomness; their broadening is enhanced due to the SOI and the strong disorder in the majority-spin channel. Magnetic anisotropy of the electronic structure for reciprocal vectors parallel and perpendicular to the magnetization direction is negligible.

MA 13.37 Tue 10:15 P1A

Spin-flip Probabilities in Concentrated and Diluted Ferromagnetic Semiconductors — •Gerald Rosenthal and Wolfgang Nolting — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin

We present an exact Green's function study of the electronic energy spectrum of a ferromagnetic semiconductor at T = 0K within the framework of the single-band as well as multi-band Kondo-lattice model. Main focus is put on quasiparticle densities of states, dispersion relations and spin-flip probabilities. The spectrum decomposes into a scattering part (magnon emission) and a quasiparticle part (magnetic polaron). The spin-flip oscillation period of the magnetic polaron can quantitatively be determined. Furthermore, the influence of disorder (diluted ferromagnetic semiconductors) on the energy spectrum and spin-flip probabilities will be discussed.

MA 13.38 Tue 10:15 P1A

Investigation of the valence states of $Fe_{1-x}Cu_xCr_2S_4$ by photoelectron spectroscopy — •Christian Taubitz[1], Michael Raekers[1], Vladimir Tsurkan[2], and Manfred Neumann[1] — [1]Universität Osnabrück, Fachbereich Physik, Barbarastraße 7, D-49069 Osnabrück, Germany — [2]Institute of Applied Physics, Academy of Science of Moldova, Kishinev MD 2028, Republic of Moldova

Spinel compounds of $Fe_{1-x}Cu_xCr_2S_4$ have attracted much attention since the discovery of a very large negative magnetoresistance (MR) effect. The valencies of Fe, Cu and Cr have been a long-standing issue in the attempt to understand the magnetic and electric properties of these compounds. In the region $0 \leq x \leq 0.5$ the Lotgering model predicts Fe to be in a mixed valence state between Fe^{2+} and Fe^{3+}. For x=0.5 all Fe-ions are assumed to be trivalent. Mössbauer measurements confirm this model, however investigations with XAS and XPS show Fe to stay in a divalent state for $0 \leq x \leq 0.5$. We show XAS, XPS and XMCD measurements of single crystalline $Fe_{0.5}Cu_{0.5}Cr_2S_4$ and the first XPS measurements of $Fe_{1-x}Cu_xCr_2S_4$ single crystals for $x>0.5$. Our results indicate no ion valency change to be present in $Fe_{1-x}Cu_xCr_2S_4$ over the whole Cu concentration range. When the surface of $Fe_{0.5}Cu_{0.5}Cr_2S_4$ is oxidised we find Fe^{3+} in a paramagnetic state. We discuss our results in view of Mössbauer measurements and theoretic models, and give possible explanations for the contradictory results.

MA 13.39 Tue 10:15 P1A

Electronic structure of $MnZnFe_2O_4$ spinel ferrite — •S. Soliman[1], A. Elfalaky[2], and Claudia Felser[1] — [1]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55099 Mainz — [2]Department of Physics, Faculty of Science, Zagazig University, Zagazig, Egypt

To fabricate materials with specific characteristics, the electronic structure of these materials should be comprehensively inspected against different conditions and circumstances. Circumstances such as chemical doping, valency of the ions, sites position, etc. might have significant modification to the band structure. Full potential linearized augment plane wave method (FP-LAPW) has been applied to calcu-

late the electronic band structure of $MnZnFe_2O_4$. According to the calculations, the semiconducting parameters were predicted in terms of exchange of Mn and Zn ion substitution.

The authors gratefully acknowledge financial support by the DfG (Research Unit 559).

MA 13.40 Tue 10:15 P1A

Electronic structure of $MnFe_2O_4$ spinel ferrite — •S. Soliman[1], A. Elfalaky[2], and Claudia Felser[1] — [1]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55099 Mainz — [2]Department of Physics, Faculty of Science, Zagazig University, Zagazig, Egypt

Full potential linearized augment plane wave method (FP-LAPW) has been exploited to calculate the electronic band structure of Mn Fe_2O_4 spinel ferrite. From the calculations, the crystal structure, position of ionic occupation within the unit cell will be imparted. Some mechanical characterization were revealed. In addition, the semiconducting parameters, density of states magnetic parameters will also be evaluated and compared with the available experimental and theoretical data.

The authors gratefully acknowledge financial support by the DfG (Research Unit 559).

MA 13.41 Tue 10:15 P1A

Magneto-optical spectroscopy of europium telluride and europium hydride — •Bodo Lobbenmeier, Helge Schröter, Peter Clodius, and Joachim Schoenes — Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany

Magneto-optical measurements on EuTe and EuH_2 have been used to investigate the electronic properties of the highly localized 4-f electrons of europium, i.e. the transition from the 4-f to the 5-d state. Since a magnetic transition from a canted antiferromagnetic to a spin-aligned phase is expected near 7 T in EuTe, the magnetic field dependencies have been measured up to 10 T. The Kerr spectroscopic investigations have been made in the energy range from 1.8 eV to 4.3 eV. The spectra for EuTe have been compared with data obtained for EuH_2 which has a similar gap than EuTe. This films of EuH_2 have been grown by pulsed laser deposition and show a transition to a ferromagnetic phase at 18 K.

MA 13.42 Tue 10:15 P1A

Curie point singularity in (Ga,Mn)As — •Vit Novak, Kamil Olejnik, Miroslav Cukr, Petr Vasek, Zbynek Soban, and Tomas Jungwirth — Institute of Physics AS CR, Cukrovarnicka 10, 162 53 Prague, Czech Republic

A striking cusp-like singularity has been found in the temperature derivative of resistivity at the Curie point of high-quality (Ga,Mn)As ferromagnetic semiconductors [1]. The character of the anomaly is sharply distinct from the critical contribution to transport in conventional dense-moment magnetic semiconductors and is reminiscent of the singularity in transition metal ferromagnets. Applicability of the singularity to accurately determine the Curie temperature is demonstrated and compared to standard magnetometry and Arrott plot technique.

[1] V. Novak et al., Phys. Rev. Letters 101, 077201 (2008).

MA 13.43 Tue 10:15 P1A

Suppression of resistivity due to thermal treatment of SnO_2 thin films — •Ali Awada[1], Dirk Menzel[1], Joachim Schoenes[1], Frank Ludwig[2], and Meinhard Schilling[2] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [2]Institut für Elektrische Messtechnik und Grundlagen der Elektrotechnik, TU Braunschweig, Germany

In the field of diluted magnetic semiconductors, transition metal doped oxides have attracted much interest because of a Curie temperature which is beyond 300 K. Among these materials SnO_2 is a promising host material for spintronic applications due to its low electrical resistivity despite a high optical transparency. Conductivity measurements of sputtered SnO_2 thin films show a resistivity in a wide range from 0.2 to 80 Ωcm at room temperature depending on the preparation parameters. The stoichiometry of the SnO_2 plays a crucial role since the conductivity of the tin dioxide is presumably determined by donor levels originating from oxygen vacancies [1]. In order to exert influence on the amount of defects the films were annealed after deposition. In comparison to the as-grown samples a suppression of the resistivity due to the thermal treatment by a factor of more than 10 is observed. Since it is assumed that the ferromagnetic exchange is mediated via free charge carriers in the sense of a magnetic polaron the tuning of the electrical properties is a key issue towards diluted magnetic semiconductors with large ordered moments and high Curie temperatures.

[1] D. Menzel, A. Awada, H. Dierke, J. Schoenes, F. Ludwig, and M. Schilling, J. Appl. Phys. **103**, 07D106 (2008).

MA 13.44 Tue 10:15 P1A

Ferromagnetic order above room temperature in cubic Y-stabilized ZrO_2 by Fe-implantation — •Monika Kotzian, Dirk Menzel, and Joachim Schoenes — Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany

Diluted magnetic oxides have attracted much interest when room-temperature ferromagnetism was observed e. g. in transition metal doped TiO_2 and SnO_2. Recently, ferromagnetic order with Curie temperatures far above 300 K was also predicted in ZrO_2 when it is doped with magnetic transition elements [1]. For an experimental verification of this prediction single crystalline Y-stabilized ZrO_2 was doped with Fe using the ion-implantation technique at high doses leading to Fe concentrations up to 7 at.%. This method was chosen in order to prevent the clustering of the magnetic ions. Due to the implantation the ZrO_2 crystals show a brownish color. However, the fundamental band gap of 4.08 eV, which was determined using optical spectroscopy, does not change significantly on doping within the investigated Fe concentration range. The ZrO_2 crystals doped with 7 at.% Fe order ferromagnetically with an ordered moment per Fe atom of 0.30 μ_B at 10 K and 0.25 μ_B at room temperature. Upon annealing the brownish color vanishes and the ordered moment decreases. This leads to the interpretation of a polaron-mediated magnetic exchange interaction.

[1] S. Ostanin et al., Phys. Rev. Lett. **98**, 016101 (2007).

MA 13.45 Tue 10:15 P1A

MBE growth of Fe_3O_4 films on ZnO — •Markus Paul[1,2], Nicholas Ingle[2], Andreas Müller[1], Andreas Ruff[1], Michael Sing[1], and Ralph Claessen[1] — [1]Lehrstuhl für Experimentelle Physik 4, Universität Würzburg, Germany — [2]AMPEL, University of British Columbia, Vancouver, Canada

Magnetite (Fe_3O_4) is ranked among the promising materials as spin-injector into a semiconducting host. Its ferrimagnetic behaviour with a high Curie temperature of about 850 K, the small conductivity mismatch to semiconductors and its theoretically predicted high spin polarization at E_F are very attractive for this goal. The deposition of magnetite thin fims on ZnO presents a further step towards integration of magnetic materials into semiconductor technology.

We have investigated the MBE growth behaviour and properties of Fe_3O_4 thin films on ZnO with various techniques. Growth proceeds as a mixed layer and island growth for typical film thicknesses ranging from 10 to 30 nm. LEED, RHEED and XRD results demonstrate (111) oriented deposition with an epitaxial relationship of $Fe_3O_4\langle 1\bar{1}0\rangle \| \, ZnO\langle 2\bar{1}\bar{1}\rangle$. XPS and HAXPES spectra reveal small changes in Fe and Zn chemical environments with varying probing depth. UPS measurements are in agreement with results obtained on single crystals showing no spectral weight at E_F.

MA 13.46 Tue 10:15 P1A

Searching for Intrinsic Magnetic Order in Pure ZnO Thin Films — •M. Khalid[1], M. Ziese[1], A. Setzer[1], P. Esquinazi[1], H. Hochmuth[2], M. Lorenz[2], M. Grundmann[2], D. Spemann[3], and T. Butz[3] — [1]Division of Superconductivity and Magnetism — [2]Semiconductor Physics Group — [3]Division of Nuclear Solid State Physics — Faculty of Physics and Geosciences, University of Leipzig, 04103 Leipzig.

Defect-induced room temperature ferromagnetism in oxide semiconductors has attracted wide research interest in recent years. In view of their potential spintronic and optoelectronic properties we studied the magnetic properties of pure ZnO films grown under reducing conditions. The films were grown by pulsed laser deposition onto Al_2O_3 $(11\bar{2}0)$ substrates. Substrate temperature was between room temperature and 570°C and N_2 partial pressure between 0.007 mbar and 0.3 mbar. The magnetic properties of the bare substrates and the ZnO films were investigated by SQUID magnetometry. The samples were directly clamped in straws for magnetization measurements to minimize spurious magnetic signals from the sample mounting. The Al_2O_3 substrates showed a small residual ferromagnetic-like contribution. None of the ZnO films showed reproducible ferromagnetic hysteresis significantly larger than the substrates. The purity of the ZnO films was checked by particle induced X-ray emission and iron con-

tamination between 30 and 200 μg iron per gram ZnO was detected. In conclusion, ZnO films grown under reducing N_2 atmosphere did not show any reproducible ferromagnetic contribution to the SQUID signal.

MA 13.47 Tue 10:15 P1A

Electronic and magnetic properties of doped ZnO — •Igor Maznichenko[1], Arthur Ernst[2], Sergey Ostanin[2], Markus Däne[1,3], Ingrid Mertig[1,2], Patrick Bruno[2,4], Wolfram Hergert[1], Jürgen Henk[2], Martin Lüders[3], Zdzislawa Szotek[3], and Walter Temmerman[3] — [1]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, D-06099 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [3]Daresbury Laboratory, Daresbury, Warrington WA4 4AD, Cheshire, United Kingdom — [4]European Synchrotron Radiation Facility - BP 220, F-38043 Grenoble Cedex, France

Oxides are interesting materials with a high potential for opto and spin electronics. Semiconductors based on ZnO demonstrate properties wanted for both of these applications. Its combination with the well known spacer material MgO exhibits extraordinary properties as a function of concentration. First of all, the binary alloy $Zn_{1-x}Mg_xO$ undergoes a structural phase transition from the wurtzite structure of ZnO to the rock-salt structure of MgO. Second, the band gap of the alloy changes from 3.4 eV for x=0 to 7.2 eV for x=1.

ZnO based diluted magnetic semiconductors demonstrate different magnetic properties depending on the type of dopant, its concentration and distribution. Especially important for applications is the existence of room temperature ferromagnetism.

First-principle studies were performed within the framework of the Korringa-Kohn-Rostoker method. The temperature-dependent magnetic properties were calculated by mapping onto a Heisenberg model.

MA 13.48 Tue 10:15 P1A

Universal scaling relation between Hall and longitudinal conductivity in Zn-substituted magnetite — Deepak Venkateshvaran, Andrea Nielsen, Matthias Althammer, Sebastian Goennenwein, •Matthias Opel, and Rudolf Gross — Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany

The anomalous Hall effect (AHE) in the low-conductivity ferromagnetic oxide $Fe_{3-x}Zn_xO_4$ with x = 0, 0.1, and 0.5 is investigated in this work. We used (001), (110), and (111) oriented epitaxial $Fe_{3-x}Zn_xO_4$ films deposited on MgO and sapphire substrates in different oxygen partial pressures to analyze the dependence of the AHE on crystallographic orientation, Zn content, strain state, and oxygen deficiency. Despite substantial differences in their magnetic and transport properties, a universal scaling relation between the anomalous Hall conductivity σ_{xy}^{AHE} and the longitudinal conductivity σ_{xx} is observed. Specifically, we find that $\sigma_{xy}^{AHE} \propto \sigma_{xx}^{\alpha}$ where $\alpha = 1.69 \pm 0.08$. Our results agree with a recent theoretical prediction for metallic ferromagnets in the dirty limit [2], extending the theory to materials for which hopping conduction prevails. The fact that the scaling relation is independent of crystallographic orientation, Zn content, strain state, and oxygen deficiency suggests that it is universal and does not depend on the detailed nature of the transport mechanism. This work is supported by the DFG within SPP 1157 and 1285 and by the DAAD.

References: [1] D. Venkateshvaran et al., Phys. Rev. B **78**, 092405 (2008). [2] S. Onoda et al., Phys. Rev. Lett. **97**, 126602 (2006).

MA 13.49 Tue 10:15 P1A

Optical and magnetooptical studies on manganite films — •Markus Jungbauer, Kai Gehrke, Vasily Moshnyaga, and Konrad Samwer — I. Physikalisches Institut, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The mechanism of the metal-insulator transition and CMR effect in perovskite manganites is still under debates. It was argued that Jahn-Teller polarons and phase separation play an essential role at this point. For further detailed study of these phenomena we built an experimental setup for simultaneous electric transport, optical and magnetooptical measurements on manganite thin films in the range of temperatures 20 K-400 K, magnetic fields up to H_{max}=15 kOe and photon energies $h\nu$=1.3 eV to 4 eV. Using this setup we studied three different manganite compounds: $La_{1-x}Sr_xMnO_3$, $La_{1-x}Ca_xMnO_3$ and $(La_{0.6}Pr_{0.4})_{1-x}Ca_xMnO_3$, epitaxially grown on MgO-substrates using MAD technique. The films were also characterized by X-ray diffraction and scanning tunneling microscopy. Then the optical transmission, faraday-rotation, faraday-ellipticity and coercitivity as a function of temperature and magnetic field were measured. The magnetic and electronic phase transition were visualized in optics and magnetooptics and compared with magnetotransport data.

Deutsche Forschungsgemeinschaft via SFB 602, TPA2 is acknowledged.

MA 13.50 Tue 10:15 P1A

Magnetic anisotropy of (100)- and (110)-oriented CrO_2 thin films — •Franz Czeschka[1], Daniel Rueffer[1], Sebastian T.B. Goennenwein[1], Rudolf Gross[1], Arunava Gupta[2], Christoph Bihler[3], and Martin S. Brandt[3] — [1]Walther-Meißner-Insitut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]MINT Center, Tuscaloosa, Alabama, USA — [3]Walter Schottky Institut, Technische Universität München, Garching, Germany

In the field of spintronics, ferromagnetic materials with a high spin polarization are important. A promising material in this context is the half metal chromium dioxide (CrO_2) with a spin polarization of $P \approx 98\,\%$ and a Curie temperature of $T \approx 390\,\mathrm{K}$. However, for the application a quantitative knowledge of its magnetic properties is essential.

We have determined the magnetic anisotropy of thin CrO_2 films with thicknesses ranging from 10 nm to 1.2 μm at room temperature by ferromagnetic resonance spectroscopy (FMR) both in the X-band (9.3 GHz) and in the K-band (24.125 GHz). The films were grown by chemical vapor deposition (CVD) on either (100)- or (110)-oriented TiO_2 single crystal substrates. A clear dependence of the magnetic anisotropy on the crystallographic orientation and on the CrO_2 thickness was observed. We discuss the influence of epitaxial strain on the magnetic anisotropy and compare our results to literature.

Financial support of the German Excellence Initiative via the "Nanosystems Initiative Munich (NIM)" is gratefully acknowledged.

MA 13.51 Tue 10:15 P1A

Interface and bulk magnetic properties of Laser-ablated Co_2(Mn,Fe)Si films measured by X-ray magnetic circular dichroism (XMCD) — •Michael Kallmayer, Peter Klaer, Horst Schneider, Gerhard Jakob, and Hans Joachim Elmers — Universität Mainz, Institut für Physik, D-55128 Mainz, Germany

Heusler alloys with a predicted spin-polarization of 100% at the Fermi edge are currently of great interest. One of these half metallic ferromagnets is Co_2(Mn,Fe)Si, which makes it a promising candidate for spintronic and TMR devices. For applications interface properties are of utmost importance. Using X-ray absorption spectroscopy, we measured the total electron yield (TEY), which provides a surface sensitive signal with a typical information depth of about 2-3 nm. Simultaneously, we measured the luminescence yield from the substrate. This signal integrates along the surface normal of the film and provides a bulk-like information. We investigated epitaxial films of Co_2MnSi, Co_2FeSi and $Co_2Mn_{0.5}Fe_{0.5}Si$ grown on MgO(100) via pulsed laser deposition. We find that the magnetic moments at the surface and in the bulk are similar and in good agreement with theoretical predictions. We discuss details of the spectral features in comparison with theoretical results.

MA 13.52 Tue 10:15 P1A

X-ray absorption spectroscopy of half-metallic Co_2TiZ (Z = Si, Ge and Sn) — •Peter Klaer[1], Michael Kallmayer[1], Thorsten Methfessel[1], Hans Joachim Elmers[1], Benjamin Balke[2], Joachim Barth[2], Tanja Graf[2], Gerhard Fecher[2], and Claudia Felser[2] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, D-55128 Mainz, Germany — [2]Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg-Universität Mainz, D-55099 Mainz, Germany

X-ray magnetic circular dichroism (XMCD) of core-level absorption spectra has been measured for the Heusler alloys Co_2TiZ (Z = Si, Ge, Sn and Sb) at the $L_{3,2}$-edge. Half-metallic properties have been predicted for Z = Si, Ge and Sn. Co_2TiZ samples were prepared by arc melting of stoichometric quantities of the constituents. Bulk samples were *in situ* cleaved, shortly before data acquisition, to guarantee a clean surface. We have determined the element specific spin and orbital magnetic moments from the XMCD spectrum using a sum rule analysyis. Results are compared with data from SQUID magnetometry and theory. Co and Ti show antiparallel magnetic spin moments, except for the compound containing Sb. This means that Co_2TiZ (Z = Si, Ge, Sn) is a ferrimagnet, in agreement with theory. Assuming, that the x-ray absorption spectra at the L_3-edge is proportional to the spin density of states (DOS), we calculated the spin resolved DOS function from the experimental XMCD spectra. These results are in agreement

with the predicted band structure of these materials. We also show atomically resolved STM images of the cleaved surfaces.

MA 13.53 Tue 10:15 P1A

Thin films of the Heusler compounds Co2FeAl and Co2FeAl0.6Si0.4 — •Elena Arbelo Jorge, Christian Herbort, and Martin Jourdan — Institut of Physics, Johannes-Gutenberg University, Mainz, Germany

Heusler compounds are potential candidates for showing half metallic properties (100% spin polarization) with a large band gap at the Fermi energy and a high Curie temperature above room temperature. Epitaxial thin films of the Heusler compounds Co2FeAl and Co2FeAl0.6Si0.4 were grown by rf sputtering. A study of their crystallographic structure, surface morphology and magnetization has been carried out. For Co2FeAl a B2 structure is found after annealing at 550°C. For Co2FeAl0.6Si0.4 L21 order is found after annealing at the same temperature. The crystallographic order depending on different annealing temperatures is shown. In both compounds a small tetragonal distortion is observed. The surface morphology of each compound is also analysed and compared. Magnetization measurements made in a Quantum Design SQUID magnetometer show a magnetic moment of 4.86μB/f.u and 4.47μB/f.u for Co2FeAl and Co2FeAl0.6Si0.4 annealed at 550°C respectively, which is 2.8% and 17,2% less than the value predicted theoretically from the Slater-Pauling rule for half metals, 5.0μB/f.u and 5.4 μB/f.u, respectively. The magnetic moment depending on different annealing temperatures is presented. Finally, TMR results obtained up to now are shown.

MA 13.54 Tue 10:15 P1A

Quadratic Magneto-optical Kerr Effect Magnetometry: Application to Co_2-based Heusler Compounds — •Peter Clausen, Jaroslav Hamrle, Simon Trudel, Oksana Gaier, and Burkard Hillebrands — FB Physik and Forschungszentrum OPTIMAS, TU Kaiserslauten, 67663 Kaiserslautern, Germany

In this poster, we present the results of our investigation of Co_2-based Heusler alloys using magneto-optical Kerr effect (MOKE) magnetometry. We find that in addition to the longitudinal MOKE signal, a strong quadratic MOKE signal is present.

As an example, in the first part of this poster we present our study of a series of Co_2MnSi thin films that were subjected to different annealing temperatures, which results in a variation of the degree of atomic ordering within the compound. We show the amplitude of the quadratic MOKE signal also varies as a function of annealing temperature.

In the second part, we present our new MOKE system that is capable of simultaneously measuring the linear and quadratic MOKE signals, as well as the isolated quadratic MOKE signal, in the presence of an arbitrarily aligned in-plane magnetic field.

Financial support by the DFG within the Forschergruppe 559 "Neue Materialien mit hoher Spinpolarisation"is gratefully acknowledged.

MA 13.55 Tue 10:15 P1A

***Ab-initio* calculations of MnO in different crystal structures and magnetic orderings** — •Andreas Schrön, Claudia Rödl, Jürgen Furthmüller, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Antiferromagnetic transition-metal oxides (TMOs) are materials of great interest for applications in new magnetic materials (e.g. dilute magnetic semiconductors) and spintronics. There have been a couple of – theoretical as well es experimental – studies on the ground-state properties of MnO, but only few including also crystal structures different from the experimental rock-salt structure.

We present an *ab-initio* study of structural, electronic, and magnetic properties of MnO using density-functional theory (DFT). The results obtained within the generalized-gradient approximation (GGA) are compared with findings taking into account an additional on-site interaction U (GGA+U) and results using the non-local hybrid HSE03 exchange-correlation functional. Besides the rock-salt structure, which is the natural ground-state structure of MnO, we focus especially on the properties of MnO crystallizing in wurtzite structure, which is the ground-state structure of e.g. ZnO, a potential host material for dilute magnetic semiconductors. We present our recent results considering six different magnetic orderings for both crystal structures, respectively, and compare them with experimental and, as far as available, other theoretical data.

MA 13.56 Tue 10:15 P1A

Ab initio studies of structural, electronic and magnetic properties of pure and doped CoO — Dmitry I. Bazhanov[1], •Pavel A. Ignatiev[2], Nikolay N. Negulyaev[3], and Valeri S. Stepanyuk[2] — [1]Faculty of Physics, Moscow State University, 119899 Moscow, Russia — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [3]Physics Department, Martin-Luther-University Halle-Wittenberg, 06099 Halle, Germany

Transition metal oxides attract much attention last years due to wide range of possible applications in micro- and magneto-electronics. A particular interest is drawn to the transition-metal oxides doped by another 3d elements. A classical example of such a system is transition-metal doped ZnO, a dilute semiconductor with coexisting magnetic, piezoelectric, optical and semiconducting properties.

We present study of pure and doped CoO with the NaCl crystal structure and type-II-fcc antiferromagnetic order. By means of pseudopotential and full-potential plane wave ab initio codes we calculate the equilibrium crystal structure of CoO, as well as variations of magnetic and electronic properties of CoO introduced by the strain. Dopants are then inserted into the CoO supercell consisting of 108 atoms. Structural relaxations caused by doping of Fe, Ni, Cu and Zn atoms are determined. Fe and Ni are found to align ferromagnetically with Co atoms in the same {111}-sheet. Nonmagnetic Cu inserted into CoO gets significant magnetic moment. Analysis of our results revealed that Ni and Cu dopants most likely do not interact with each other, contrary to the strong magnetic interaction between Fe atoms.

MA 13.57 Tue 10:15 P1A

Elastic properties of single crystal manganites — •Markus Michelmann[1], Dennis Bedorf[1], Emanuel Malek[2], Thomas Koeppe[1], Lakshmana Sudheendra[1], Vasily Moshnyaga[1], and Konrad Samwer[1] — [1]I. Physikalisches Institut, Universität Göttingen — [2]Cambridge University

We have studied the metal-insulator-transition in single crystal perovskite manganites by measurements of velocity of ultrasound waves. The single crystals of $La_{1-x}Ca_xMnO_3$ (LCMO), $Nd_{1-x}Ca_xMnO_3$ (NCMO) and $Pr_{1-x}Ca_xMnO_3$ (PCMO) were grown by zone melting technique. For LCMO the dependence of shear modulus on the temperature (40-280K) and magnetic field (0-5T) was measured by means of runtime of shear waves. The results show, that metal-insulator-transition is accompanied by a decrease of the stiffness, which as well can be driven by the temperature and/or the magnetic field. A comparison with the data of NCMO and PCMO crystals will be done.

Deutsche Forschungsgemeinschaft via SFB 602, TPA2 is acknowledged

MA 13.58 Tue 10:15 P1A

Atomic-scale images of the paramagnetic insulating state in a $Pr_{0.68}Pb_{0.32}MnO_3$ single crystal — •Sahana Roessler[1], Steffen Wirth[1], Frank Steglich[1], B Padmanabhan[2], Suja Elizabeth[2], and H. L. Bhat[2] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnizer Straße 40, 01187, Dresden, Germany — [2]Department of Physics, Indian Institute of Science, Bangalore 560012, India

Scanning tunneling microscopy and spectroscopy (STM/S) have been performed on a colossal magnetoresistive manganite $Pr_{0.68}Pb_{0.32}MnO_3$ (PPMO) single crystal. In this compound, the metal-insulator transition occurs at temperature T_{MI} = 255 K[1]. STS revealed inhomogeneous maps of the zero-bias conductance with small patches of metallic clusters on a length scale of 2-3 nm only within a narrow temperature range close to but below the metal-insulator transition [2]. Here we present atomic-scale images taken at ambient temperature in the paramagnetic insulating state. The room-temperature image clearly depict the square lattice expected for the (010) suface of PPMO in a simple cubic notation. The corresponding lattice constant a_0 =3.75 ±0.6 Å is in agreement with the value determined by powder x-ray diffraction. We will also present STS results on an atomically resolved surface of PPMO.

[1] B. Padmanabhan *et al.* J. Magn. Magn. Mat. **307** 288 (2006). [2] S. Rößler *et al.* Euro. Phys. Lett. **83** 17009 (2008).

MA 13.59 Tue 10:15 P1A

Ferromagnetic Signals in Nominally Non-magnetic Oxide Single Crystals — •M. Ziese[1], A. Setzer[1], P. Esquinazi[1], D. Spemann[2], and A. Poeppl[3] — [1]Division of Superconductivity and Magnetism — [2]Division of Nuclear Solid State Physics — [3]Division of Magnetic Resonance of Complex Quantum Solids — Faculty of Physics

and Geosciences, University of Leipzig, 04103 Leipzig.

Defect-induced room temperature ferromagnetism in oxide semiconductors has attracted wide research interest in recent years. It appears that ferromagnetic order can be induced either in the bulk, when a narrow impurity band is present, or at the surface due to the lowering of the symmetry. In this work the magnetic properties of MgO, $MgAl_2O_4$, $SrTiO_3$, $LaAlO_3$, LSAT and ZnO single crystals were investigated. These crystals show three contributions to the magnetization, namely an intrinsic diamagnetic contribution, a paramagnetic contribution due to various transition metal impurities as well as a ferromagnetic contribution. The latter shows remanent magnetization and coercive field values that are strikingly independent of the actual crystal material. The magnetization data are correlated with results from particle induced X-ray emission and electron paramagnetic resonance spectroscopy. The origin of the ferromagnetic contribution is discussed in three different scenarios: (i) as caused by ferromagnetic impurities, (ii) as related to artifacts of the SQUID magnetometer and (iii) as arising from defect-induced ferromagnetism.

MA 13.60 Tue 10:15 P1A

Structural and DFT studies on $YFeMnO_5$ — •Torsten Weissbach[1], Axel Lubk[1], Tilmann Leisegang[1], Thomas Führlich[1], Falk Wunderlich[1], Dmitri Souptel[2], Günter Behr[2], Igor Chaplygin[4], Gotthard Seifert[4], Dirk C. Meyer[1], and Sibylle Gemming[3] — [1]Institut für Strukturphysik, TU Dresden — [2]Institut für Festkörper-und Werkstoffforschung (IFW) Dresden — [3]Forschungszentrum Dresden-Rossendorf — [4]Institut für Physikalische Chemie und Elektrochemie, TU Dresden

Ferromagnetic and ferroelectric oxides of composition $REMn_2O_5$ have become known for exhibiting a coupling between those properties. On substitution of Fe in $YMn_{2-x}Fe_xO_5$, the crystal structure is conserved, but the magnetic structure changes and the ferroelectricity disappears. X-ray diffraction measurements on a series of powders with different Fe content were employed to inspect the crystal structure whereas extended X-ray absorption fine structure measurements were done to identify the iron substitution site. Density functional theory calculations of the electronic structure for $YMnFeO_5$ were carried out using the experimentally determined crystal structure data and the FPLO-5 program. Different magnetic structures are studied to determine the type of interaction between the magnetic ions.