MA 27: Half-metals and Oxides (jointly with TT)

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

MA 27.1 Wed 9:30 EB 202

Scalable Exchange Bias Effect in $La_{0.66}Sr_{0.33}MnO_{3-x}/SrTiO_3$ thin films — •Daniel Schumacher[1], Alexandra Steffen[1], Jörg Voigt[1], Jürgen Schubert[1], Hailemariam Ambaye[2], Valeria Lauter[2], John Freeland[3], and Thomas Brückel[1] — [1]Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — [3]Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, USA

We present an Exchange Bias (EB) effect of controllable size in $La_{0.66}Sr_{0.33}MnO_{3-x}/SrTiO_3$ (LSMO/STO) thin films. Samples have been prepared by Pulsed Laser Deposition and High-Pressure Sputter Deposition in oxygen atmosphere at different oxygen pressures. Increased out-of-plane lattice parameters of the LSMO layers and reduced Curie temperatures indicate oxygen deficiencies in the samples grown at lower oxygen pressures. Whereas the growth at high pressures does not lead to an EB effect, we found an increase of the EB and the coercive fields with decreasing oxygen pressure. Polarized Neutron Reflectometry and X-ray Resonant Magnetic Scattering has been performed to analyze the magnetic depth profile. A layer without net magnetization in LSMO at the interface to STO has been detected in an exchange-biased sample, but not in the non-exchanged-biased one. Hence, an antiferromagnetic structure in this region could be present, which causes the EB effect in this system. A possible explanation is given based on the phase diagram of LSMO.

MA 27.2 Wed 9:45 EB 202

Temperature-dependent magnetic properties of cubic $La_{0.7}Sr_{0.3}MnO_3/SrRuO_3$ from first principles — •Danny Böttcher[1,2], Arthur Ernst[1], Igor Maznichenko[2], and Jürgen Henk[1,2] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Martin Luther University Halle-Wittenberg, Halle, Germany

Heterostructures of an antiferromagnetic manganite and an itinerant ferromagnet, e. g. $La_xSr_{1-x}MnO_3$ combined with $SrRuO_3$, exhibit fascinating properties due to the interplay between exchange coupling, magnetocrystalline anisotropy, and interfacial quality [1].

We report on a first-principles study of cubic $La_{0.7}Sr_{0.3}MnO_3$/-$SrRuO_3$ and on Monte Carlo simulations in the framework of a classical Heisenberg model. The exchange parameters of the latter as well as the magnetocrystalline anisotropy constants are calculated from first principles. The spin Hamiltonian includes in addition the dipole-dipole interaction and an external magnetic field.

We focus on the temperature dependency of magnetization and hysteresis loops of this exchange-bias system. In particular, correlation functions reveal atom-resolved magnetic properties at the interfaces.

[1] M. Ziese *et al.*, Phys. Rev. Lett. **104** (2010) 167203.

MA 27.3 Wed 10:00 EB 202

Strained thin films of $LaSrMnO_4$ grown by Pulsed Laser Deposition — •Mehran Vafaee Khanjani, Philipp Komissinskiy, Aldin Radetinac, Thorsten Bitsch, and Lambert Alff — Institute for Materials Science, Technische Universität Darmstadt, 64287 Darmstadt, Germany

It is well known that charge and orbital ordering (COO) phenomena occur in a variety of manganese oxide compounds. In the single-layered Ruddlesden-Popper manganite $La_{1-x}Sr_{1+x}MnO_4$, the COO has been observed for $x = 0.5$ which is strongly related to the lattice constants ($a = 3.86$, $c = 12.42$ Å) and Mn-O bond length [1-3]. Strain in thin films affects the structure parameters and consequently the COO. For the first time, we report on the thin film deposition of $LaSrMnO_4$ using pulsed laser deposition. X-ray diffraction reveals the growth of either fully strained or totally relaxed thin films on (110) $NdGaO_3$ and (001) $LaSrAlO_4$ substrates. Such strained thin films with in-plane lattice constants close to the $x = 0.5$ compound ($a = 3.86$, $c = 12.87$) will be the base to study the strain dependence of orbital ordering e.g. by X-ray absorption techniques. The authors would like to thank DPG GK 1035.

[1] D. Senff et al, Phys. Rev. B 71, 024425 (2005). [2] R. Mahesh et al, J. Solid State Chem. 122, 448 (1996) [3] C. S. Hong et al, Chem. Mater. 13, 945 (2001).

MA 27.4 Wed 10:15 EB 202

Magnetic characterization of ferromagnetic LSMO layers on STO grown by different methods — •Martin Wahler[1], Christian Eisenschmidt[1], Nico Homonnay[1], Ionela Vrejoiu[2], Alek Dediu[3], Vasily Moshnyaga[4], and Georg Schmidt[1] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, von-Danckelmann-Platz 3, 06120 Halle, Germany — [2]Max Planck Institute of Microstructure Physics, 06120 Halle, Germany — [3]Institute of Nanostructured Materials, ISMN-CNR, 40129 Bologna, Italy — [4]I. Physikalisches Institut, Friedrich-August-Universität Göttingen, 37077 Göttingen, Germany

$La_xSr_{(1-x)}MnO_3$ is widely used as a ferromagnetic electrode for example in organic spintronics. Its epitaxial thin films are well established in oxide heterostructures. For best performance in spintronics applications it is necessary to deposit layers with perfect crystallinity and good control of ferromagnetism and anisotropy. We have investigated LSMO thin films deposited on Strontiumtitanate by various methods namely pulsed laser deposition (PLD), pulsed plasma deposition (PPD) and metalorganic aerosol deposition (MAD). All samples show high crystalline quality as confirmed by X-ray diffractometry and reflectometry. SQUID magnetometry shows that in saturation the layers deposited by PLD and PPD yield similar magnetization values, while the value obtained from MAD samples is higher. Curie temperatures range from 280 K for PPD to $>$ 300 K for PLD and MAD grown samples. The anisotropy as determined by ferromagnetic resonance is uniaxial in plane at room and biaxial at lower temperatures.

MA 27.5 Wed 10:30 EB 202

Fundamental ab-initio studies of $SrRuO_3$, $SrTcO_3$ and $Sr_3Ru_2O_7$ including the observation of [001] surface properties concerning $Sr_3Ru_2O_7$ — •Marcel Hieckel[1,2], Cesare Franchini[3], Jiangang He[3], Florian Mittendorfer[1], Josef Redinger[1], and Raimund Podloucky[2] — [1]Institute of Applied Physics, Vienna University of Technology — [2]Institute for Physical Chemistry, Univ. Vienna — [3]Department for Computational Materials Physics, Univ. Vienna

Oxide perovskite materials attracted enormous attention because of a variety of intriguing physical properties. In this context, we present results of density functional theory (DFT) calculations for the bulk materials $SrRuO_3$, $SrTcO_3$ and $Sr_3Ru_2O_7$ and the [001] surface of $Sr_3Ru_2O_7$. For the exchange-correlation functional the generalized gradient approximation of Perdew-Burke-Ernzerhof [1] was used and further studies were made with post-DFT concepts such as hybrid functional [2] and GW approaches [3]. Structural, electronic and magnetic properties were investigated for all the systems. Furthermore, simulations of scanning tunneling microscopy experiments [4] were performed for the clean as well as the CO-covered Sr3Ru2O7 [001] surface.

Work supported by the Austrian FWF, project Nr. F4511-N16.

[1] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 77, 3865 (1966). [2] A. V. Krukau et al., J. Chem. Phys. 125, 224106 (2006). [3] L. Hedin, Phys. Rev. 139, A796 (1965). [4] J. Tersoff and D. R. Hamann, Phys. Rev. B 31, 805 (1985).

15 min. break

MA 27.6 Wed 11:00 EB 202

p-Electron Magnetism in anion doped $BaTiO_{3-x}X_x$ (X=C,N,B). — Christoph Gruber[1], •Pedro Osvaldo Bedolla Velazquez[1], Josef Redinger[1], Peter Mohn[1], and Martijn Marsman[2] — [1]Vienna University of Technology, Gusshausstrasse 25-25a/134, 1040 Vienna, Austria — [2]University of Vienna, Sensengasse 8/12 1090 Vienna, Austria

We present VASP calculations using the HSE functional for carbon, nitrogen, and boron doped $BaTiO_{3-x}X_x$ (X=C,N,B). We calculate a 40-atom supercell and replace one oxygen atom by C,N, or B. For all three substituents we find a magnetically ordered groundstate which is insulating for C and N and halfmetallic for B. The changes in the electronic structure between the undoped and the doped case are dominated by the strong crystal field effects together with the large band splitting for the impurity p-bands. Using an MO picture we give an explanation for the pronounced changes in the electronic structure between the insulating non-magnetic state and the as well insulating

magnetic state for doped $BaTiO_3$. p-element doped perovskites could provide a new class of materials for various applications ranging from spin-electronics to magneto-optics.

MA 27.7 Wed 11:15 EB 202

Magnetic and Electrical Properties of the possibly Antiferromagnetic Half-metal Double Perovskite La_2CrWO_6 — •Mehran Vafaee Khanjani, Philipp Komissinskiy, Mehrdad Baghaie Yazdi, Anastasiya Kolchynska, and Lambert Alff — Institute for Materials Science, Technische Universität Darmstadt, 64287 Darmstadt, Germany

The combination of a magnetic ion (B-site) and a non-magnetic ion (B'-site) in double perovskites ($A_2BB'O_6$) can lead to an *induced* magnetic moment at the non-magnetic site [1-3]. Therefore, double perovskites are hot candidates in the search for compensated antiferromagnetic half-metals (AFM-HMs) which are considered to be useful for spintronics, supplying on the one hand, fully spin-polarized electrons, and on the other hand due to the antiferromagnetic configuration, they are magnetically stable. Following band structure calculations [4] and a simple ionic picture, La_2CrWO_6 is an AFM-HM candidate. However, as bulk material this compound is thermodynamically unstable. One way of synthesizing such a material is a thin film approach forcing W into a very unusual W^{3+} state. To our knowledge, we have synthesized for the first time La_2CrWO_6 by pulsed laser deposition. Crystal structure, magnetic and electrical properties are presented. The Authors would like to thank the DFG GK 1035.

[1] K. L. Kobayashi et al, Nature 395, 677 (1998). [2] Y. Krockenberger et al, Phys. Rev. B 75, 020404(R) (2007). [3] A. Winkler et al, New J. Phys. 11, 073047 (2009). [4] V. Pardo et al, Phys Rev B 80, 054415 (2009).

MA 27.8 Wed 11:30 EB 202

Cation distributions and its influence on magnetostrictive properties in inverse spinel ferrites $CoFe_2O_4$ and $NiFe_2O_4$ — •Daniel Fritsch and Claude Ederer — School of Physics, Trinity College Dublin, Ireland

Spinel ferrites $CoFe_2O_4$ (CFO) and $NiFe_2O_4$ (NFO) are both insulating ferrimagnetic oxides with a high magnetic ordering temperature and large saturation magnetisation. Moreover, CFO is a highly magnetostrictive material, i.e., it shows a large length change when exposed to a magnetic field.

The spinel structure consists of two magnetic sublattices, namely A- and B-sublattice, which in the *normal* spinel structure are solely occupied by one of the two cation species. An increasing exchange between the two cation species leads to the *inverse* spinel structure where two cation species are distributed over the B-sublattice. These different possible cation distributions over the B-sublattice strongly influence the total energy of these materials [1].

It has already been shown that density functional theory (DFT) calculations together with the Hubbard "+U" approach provide reliable insight in the structural and magnetic properties of these materials [2]. Here we present DFT total energy calculations for CFO and NFO with different possible cation distributions over the B-sublattice and their influence on the magnetostrictive properties. These results are compared to available experimental data.

[1] D. Fritsch and C. Ederer, Appl. Phys. Lett. **99**, 081916 (2011).
[2] D. Fritsch and C. Ederer, Phys. Rev. B **82**, 104117 (2010).

MA 27.9 Wed 11:45 EB 202

Zinc ferrite - magnetic thin films with highly tunable conductivity — •Kerstin Brachwitz, Katja Mexner, Michael Lorenz, Francis Bern, Michael Ziese, Pablo Esquinazi, and Marius Grundmann — Institut für Experimentelle Physik II, Universität Leipzig, Germany

Zinc ferrite ($ZnFe_2O_4$) has been investigated in several studies, especially because of its promising magnetic properties. However, also the electrical properties are remarkable and important for the application of $ZnFe_2O_4$ in spin filters and magnetic tunnel junctions. In this regard, $ZnFe_2O_4$ thin films were grown by pulsed-laser deposition. The substrate temperature T_S and the oxygen partial pressure $p(O_2)$ were varied for different samples in the range of $430°C \leq T_S \leq 730°C$ and $5 \cdot 10^{-5} \leq p(O_2) \leq 10^{-2}$ mbar, respectively.

The electrical conductivity of the resulting $ZnFe_2O_4$ films can be tuned over 7 orders of magnitude in a range from 10^{-5} to 10^2 S/m by varying T_S [1]. The conductivity of such thin films is thermally activated with activation energies between 70 and 120 meV. The free carrier concentration and their mobility were determined by anomalous Hall effect measurements. Thin films with the largest conductivity exhibit values of about $n = 10^{20}\,cm^{-3}$ and $\mu = 0.07\,cm^2/Vs$.

Furthermore, the structural properties were investigated by X-ray diffraction. These measurements revealed an increasing *a*-lattice constant with increasing conductivity, indicating a disorder- and vacancy-induced conduction mechanism.

[1] M. Lorenz *et al.*, Phys. Status Solidi RRL **5**, 438 (2011)

MA 27.10 Wed 12:00 EB 202

Giant spontaneous magnetostriction in $FeTiO_3$: effects of repulsive dipole-dipole interactions — •Michalis Charilaou[1,2], Denis Sheptyakov[3], Jörg F Löffler[2], and Andreas U Gehring[1] — [1]Earth and Planetary Magnetism, Department of Earth Sciences, ETH Zurich, 8092 Zurich, Switzerland — [2]Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — [3]Laboratory for Neutron Scattering, Paul Scherrer Institute, 5232 Villigen, Switzerland

We present neutron diffraction data and magnetic susceptibility measurements of $FeTiO_3$ ilmenite at temperatures of 1.9 K < T < 300 K. The magnetic susceptibility shows typical antiferromagnetic behavior with a long-range ordering at the Néel temperature $T_N = 58(1)$ K. The magnetic peaks of the neutron diffraction patterns reveal a canted antiparallel spin configuration along the c axis of the R-3 structure. The lattice dimensions decrease with decreasing temperature, but upon the onset of order the c-dimension grows strongly, and at T = 1.9 K exhibits a spontaneous magnetostriction of 2.46(9) 10^{-3}. The observations are interpreted as the result of repulsive dipole-dipole interactions between neighboring Fe-rich layers and the onset of spin-orbit coupling at T_N.