MA 14: Magnetic Half Metals and Oxides

Time: Tuesday 10:30–13:15 Location: EB 202

MA 14.1 Tue 10:30 EB 202

Onset of magnetic order in 3d transition metal oxides — •Guntram Fischer[1], Ian Hughes[2], Markus Däne[3], Arthur Ernst[3], Wolfram Hergert[1], Julie B. Staunton[2], Martin Lüders[4], Zdzislawa Szotek[4], and Walter Temmerman[4] — [1]Institute of Physics, MLU Halle-Wittenberg, Von-Seckendorff-Platz 1, 06120 Halle — [2]Department of Physics, University of Warwick, Coventry, CV4 7AL, UK — [3]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle — [4]Daresbury Laboratory, Daresbury, Warrington, WA4 4AD, UK

The finite temperature magnetic properties of 3d transition metal oxides (TMO) will be discussed based on ab initio methods. Self-interaction corrections are taken into account in a local implementation (LSIC) within the KKR multiple-scattering theory.[1] The calculation of exchange parameters by means of the magnetic force theorem [2] allows us to calculate the Neel temperatures via Mean Field Approximation, Random Phase Approximation and Monte Carlo simulations. The use of LSIC-KKR in combination with the disordered local moment (DLM) method [3] opens up the alternative to calculate the transition temperatures without any mapping to a Heisenberg model.The results of the different approaches will be compared and discussed. The dependence of the transition temperatures on the lattice constant and the magnon spectra of the TMO will be discussed as well. - [1] M. Lüders et al. Phys. Rev. B, 71, 205109 (2005), [2] A.A. Liechtenstein et al. JMMM, 67, 65 (1987), [3] Gyorffy et al., J. Phys. F: Met. Phys. 15, 1337 (1985)

MA 14.2 Tue 10:45 EB 202

Origin of magnetism in hematite-ilmenite system from first principles — •Hasan Sadat Nabi and Rossitza Pentcheva — Department of Earth and Environmental Sciences, University of Munich, Theresienstr. 41, 80333 Munich, Germany

The high remanent magnetization measured in exsolutions of the canted antiferromagnet hematite (Fe_2O_3) and room-temperature paramagnet ilmenite ($FeTiO_3$) has received considerable attention in recent years[1]. To resolve the microscopic origin of magnetism at the interface of hematite and ilmenite, we have performed density functional theory calculations, varying systematically the concentration, distribution, and charge state of Ti (Fe) in a hematite (ilmenite) host. Our investigation shows that including electronic correlation within the LDA+U approach is decisive to obtain the correct magnetic ground state and band gap of the end members, α-$Fe^{3+}{}_2O_3$ and $Fe^{2+}Ti^{4+}O_3$. We find that Ti substituting for Fe^{3+} in the hematite host is not inert as commonly assumed but plays an active role in compensating the charge mismatch at the interface and the emergence of magnetism: In a single Ti layer in a hematite host, the preferred charge state is Ti^{3+}, Fe^{3+}. As soon as a thicker ilmenite-like block forms, the most favorable compensation mechanism is through Ti^{4+} and a disproportionation in the Fe contact layer in Fe^{2+}, Fe^{3+} giving first theoretical evidence for the *lamellar magnetism hypothesis* [1]. The substitution of Ti (or Fe) in Fe_2O_3 ($FeTiO_3$) leads to impurity levels in the band gap and in some cases to half-metallic behavior.
[1] Robinson, P. *et al.* Nature **418**, 517 (2002).

MA 14.3 Tue 11:00 EB 202

Investigations of the Co_2MnSi/MgO(001) heterojunction - Looking for half-metallicity — •Björn Hülsen[1], Peter Kratzer[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin — [2]Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg

Magnetic memory devices that exploit the tunneling magnetoresistance (TMR) effect depend crucially on the spin polarization of the electrode materials. Ferromagnetic half-metals make perfect electrodes leading to a (theoretically) infinite TMR ratio. The full Heusler alloy Co_2MnSi is predicted to be half-metallic and has recently been integrated in a magnetic tunnel junction[1] where a high TMR value and huge spin polarization have been measured.

Here, we use density functional theory (DFT) calculations to model an epitaxially grown Co_2MnSi/MgO(001) interface as potential TMR device. Different terminations of Co_2MnSi (stoichiometric Co- and MnSi- and non-stoichiometric Mn- and Si- planes) and different registry with respect to the insulating barrier (Mg-top, O-top, bridge, and hollow site) are investigated. For all terminations the O-top site is the stable configuration whereas the bridge site is unstable. By investigating the electronic and magnetic properties we find that the existence of the spin gap depends strongly on the termination. In most cases it is closed by interface states but in one case the half-metallicity is preserved.

[1] M. Oogane *et. al.*, J. Phys. D: Appl. Phys. **39** 834 (2006)

MA 14.4 Tue 11:15 EB 202

Magnetic anisotropy and exchange interaction in Co_2-based Heusler compounds — •Jaroslav Hamrle[1], Oksana Gaier[1], Burkard Hillebrands[1], Horst Schneider[2], Gerhard Jakob[2], Martin Jourdan[2], Yuya Sakuraba[3], Takahide Kubota[4], Mikihiko Oogane[4], and Yasuo Ando[4] — [1]FB Physik and FFSP MINAS, TU Kaiserslautern, Erwin Schrödinger-Str. 56, D-67663 Kaiserslautern, Germany — [2]Institut für Physik, Johannes-Gutenberg-Universität, D-55128, Mainz, Germany — [3]Institute of Materials Research, Tohoku University, 2-1-1 Katahira, Sendai 980-8577, Japan — [4]Graduate School of Engineering, Tohoku University, Aoba-yama 6-6-05, Sendai 980-8579, Japan

Co_2-based Heusler compounds are promising candidates to provide 100% spin polarization. We report on magnetic anisotropy, exchange interaction and magnetization reversal in Co_2FeSi, $Co_2Cr_{0.6}Fe_{0.4}Al$ (CCFA), Co_2MnSi and $Co_2MnAl_xSi_{1-x}$ Heusler compounds using Mageto-Optical Kerr effect magnetometry and Brillouin ligh scattering spectroscopy. The samples are studied as a function of sample composition, sample ordering and sample thickness. It is shown that inside ordered CCFA or Co_2FeSi films, there is a wide distribution of the internal field, smearing out the internal 4-fold anisotropy and providing a constant coercive field independent of the sample orientation. The values of the exchange stiffness constant for various Heusler compounds are presented. The project was financially supported by the Research Unit 559 "New materials with high spin polarization" funded by the DFG and by the NEDO Programm 2004/T093.

MA 14.5 Tue 11:30 EB 202

Solving the problem of structure determination in 3d transition metal based Heusler compounds. — •Benjamin Balke, Gerhard H. Fecher, Christian Blum, Lubna Basit, and Claudia Felser — Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55099 Mainz

This work reports on the structural investigation of Fe-containing, Co2-based Heusler compounds (Co_2FeZ with Z = Al, Si, Ga, Ge) using anomalous X-ray diffraction (XRD) and extended X-ray absorption fine structure spectroscopy (EXAFS). Using XRD, it was shown that Co_2FeAl crystallizes in the $B2$ structure whereas Co_2FeSi crystallizes in the $L2_1$ structure. For compounds containing Ga or Ge, the XRD technique with regular laboratory sources for excitation can not be used easily to distinguish the two structures. For this reason, EXAFS was used to elucidate the structure of these two compounds. The absorption experiments close to the K-edges of Co, Fe, Ga, and Ge indicated that both compounds crystallize in the $L2_1$ structure. Exciting the XRD at the K-edges of Co and Fe leads to anomalous X-ray scattering. The dependence of the scattering parameters on the energy close to the absorption edges was used to identify the $L2_1$ structure of the Ga and Ge containing compounds unambiguously. The applicability of the techniques on nano-scaled materials will be demonstrated for the example of Co_2FeGa nano-particles with sizes of below 25 nm.

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

MA 14.6 Tue 11:45 EB 202

Modification of structural and magnetic properties of Co_2FeSi and Co_2MnSi Heusler compounds by ion irradiation — •Oksana Gaier[1], Jaroslav Hamrle[1], Burkard Hillebrands[1], Horst Schneider[2], Gerhard Jakob[2], Yuya Sakuraba[3], Sumito Tsunegi[3], Mikihiko Oogane[3], Yasuo Ando[3], Jürgen Fassbender[4], Bernhard Reuscher[5], Alexander Brodyanski[5] und Michael Kopnarski[5] — [1]TU Kaiserslautern, 67663 Kaiserlautern — [2]Johannes-Gutenberg-Universität, 55128 Mainz — [3]Tohoku University, Sendai 980-8579, Japan — [4]Forschungszentrum Dresden-Rossendorf, 01328 Dresden — [5]IFOS, TU Kaiserslautern, 67663 Kai-

serslautern

Spin polarization in Co_2FeSi and Co_2MnSi Heusler compounds is believed to be very sensitive to the degree of $L2_1$ order. In thin films, the transition from the disordered to the $L2_1$ ordered phase is usually achieved by an annealing step after film deposition. This procedure, however, is not suitable if local modifications of crystallographic properties are required. In such a case irradiation with keV ions is a convenient tool as reported for FePd and FePt films. Here, we report on the dependence of structural and magnetic properties of thin Co_2FeSi and Co_2MnSi films on the irradiation by 30 keV He^+ and Ga^+ ions.

The project was financially supported by the Research Unit 559 "New materials with high spin polarization"funded by the DFG, by the NEDO International Joint Research Grant Programm 2004/T093 and by the Stiftung Rheinland-Pfalz für Innovation.

MA 14.7 Tue 12:00 EB 202

Magnetism in Re-based ferrimagnetic double perovskites — Andreas Winkler[1], Narendirakumar Narayanan[1], Daria Mikhailova[1], Helmut Ehrenberg[2], Hartmut Fuess[1], Fabrice Wilhelm[3], Andrei Rogalev[3], and •Lambert Alff[1] — [1]Institut für Materialwissenschaft, TU Darmstadt — [2]IFW Dresden — [3]ESRF, Grenoble, France

We have investigated spin and orbital magnetic moments of the Re $5d$ ion in the double perovskites A_2FeReO_6 (A = Ba, Sr, Ca) by X-ray magnetic circular dichroism (XMCD) at the Re $L_{2,3}$ edges. In these ferrimagnetic compounds an unusually large negative spin and positive orbital magnetic moment at the Re atoms was detected. The presence of a finite spin magnetic moment in a 'non-magnetic' double perovskite as observed in the double perovskites Sr_2ScReO_6 proves that Re has also a small, but finite *intrinsic* magnetic moment. These results further support a kinetic energy driven exchange model for the ferrimagnetic double perovskites. We further show for the examples of Ba and Ca that also the usually neglected alkaline earth ions undoubtedly also contribute to the magnetism in the ferrimagnetic double perovskites.

MA 14.8 Tue 12:15 EB 202

Ab initio cluster calculations of Co^{3+} spin states in $RBaCo_2O_{5.5}$ (R=Ho,Gd) — Luidmila Siurakshina[1,2], •Beate Paulus[3], and Viktor Yushankha[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden — [2]Joint Institute for Nuclear Research, 141980 Dubna, Russia — [3]Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin

We investigated the different Cobalt spin-states of two members of oxygen-deficient perovskites $RBaCo_2O_{5.5}$(R=Ho, Gd). These materials are promising compounds for ionic conductors necessary for solid oxide fuel cells. The studies involve ab-initio calculations for clusters at the multi-reference configuration interaction level to describe all spin-states at equal footing. The emphasis is made on the peculiar behaviors of the trivalent ions $Co^{3+}(3d^6)$ in an octahedral and a pyramidal oxygen coordinations, which is related to a structural first-order phase transition in both compounds. Relative energy positions of low spin ($S = 0$), intermediate spin ($S = 1$) and high spin ($S = 2$) cluster electron configurations are calculated for the low- and high-temperature lattice structures of $RBaCo_2O_{5.5}$. The calculated results and experimental structural data are analyzed and comprised in a model that enables us to catch the most prominent features common to the phase transition in both compounds.

MA 14.9 Tue 12:30 EB 202

Influence of MBE growth rate on the structural and magnetic properties of epitaxial NiMnSb layers — •Florian Lochner, Peter Bach, Charles Gould, Christian Kumpf, Georg Schmidt, and Laurens W. Molenkamp — Physikalisches Institut (EP3), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

NiMnSb is a promising material for application in future spintronic devices because of its expected half-metallicity and the high Curie temperature of 730 K. In addition, NiMnSb crystallizes in the C_{1b} structure [1] which is compatible to various Zincblende-type III/V semiconductors. We have shown previously that high quality NiMnSb layers can be deposited on (In,Ga)As buffer layers by molecular beam epitaxy [2]. Here we demonstrate that lowering the growth rate from 0.2178 Å/s to 0.0442 Å/s leads to changes in the structural and magnetic properties of the NiMnSb layers. While the interface flatness is reduced, as can be inferred from X-ray diffraction, the line width in ferromagnetic resonance (FMR) decreases, indicating a low damping and high magnetic quality. We will show results of samples deposited on (001) and (111) oriented InP substrates with a thin (In,Ga)As buffer which is almost lattice matched to the NiMnSb. The growth process and structural properties (including relaxation dynamics) are characterized by RHEED patterns and HRXRD measurements, respectively. The magnetic properties are investigated by MOKE and FMR. We acknowledge the support of the EU project Dynamax.

[1] R.A. de Groot et al., Phys. Rev. Lett. **50** (1983) 2024
[2] Peter Bach et al., J. Cryst. Growth **251** (2003) 323-326

MA 14.10 Tue 12:45 EB 202

The local structure of Co_2FeZ (Z=Si, Al, Ga, Ge) Heusler compounds probed by ^{59}Co NMR — •Sabine Wurmehl[1], Jürgen T. Kohlhepp[1], Henk J. M. Swagten[1], Bert Koopmans[1], Marek Wojcik[2], Christian G. F. Blum[3], Benjamin Balke[3], Gerhard H. Fecher[3], Vadim Ksenofontov[3], and Claudia Felser[3] — [1]Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands — [2]Polish Academy of Sciences, 02-668 Warszawa, Poland — [3]Johannes Gutenberg - Universität, 55099 Mainz, Germany

A thorough structural characterisation is one of the key tools in understanding the properties of spin polarised materials as the Heusler compounds Co_2FeZ with Z=(Si, Al, Ge, Ga). Spin echo nuclear magnetic resonance (NMR) spectroscopy provides a tool to probe the local structure by measuring the resonance frequencies and to probe the local hyperfine fields including the unique possibility to resolve the occupation and hyperfine fields of the neighboring shells. Thus, NMR was used to study the local (magnetic) structure of Co_2FeZ (Z=Al, Si, Ga, Ge) Heusler compounds, revealing different types of multiplet resonance lines for different types of Z atoms. The observed splitting of the resonance lines originates from different local environments of the ^{59}Co nuclei. Analysis of the spectra yields the corresponding resonance frequencies and hyperfine magnetic fields as well as the spacing between consecutive resonance lines which leads to macroscopic structural models for the investigated Co_2FeZ Heusler compounds with Z=(Si, Al, Ge, Ga). (This work is funded by the DFG (FG 559) TP1. SW gratefully acknowledges funding by DFG in project WU 595/1-1.)

MA 14.11 Tue 13:00 EB 202

Exotic, anionogenic magnetism in the alkali sesquioxide Rb_4O_6. — •J. Winterlik[1], G. H. Fecher[1], C. Felser[1], C. Mühle[2], M. Jansen[2], L. M. Sandratskii[3], and J. Kübler[4] — [1]Institut für Anorganische und Analytische Chemie, Johannes Gutenberg - Universität, 55099 Mainz — [2]Max - Planck - Institut für Festkörperforschung, 70569 Stuttgart — [3]Max - Planck - Institut für Mikrostrukturphysik, 06120 Halle — [4]Institut fü Festkörperphysik, Technische Universität, 64289 Darmstadt

The chemical formula Rb_4O_6 implies a simple alkali oxide. Taking into account its black color and its mixed valency, things get much more complicated in the case of this so-called rubidium sesquioxide. Up to the present, an accurate description of its electronic structure has not yet been provided. The investigation of temperature dependent magnetic properties indicated p-electron based magnetic frustration. Here, we present experimental results that confirm this proposed magnetic frustration. In addition, we provide a theoretical model for the exceptional crystal of Rb_4O_6. The introduction of electron-electron correlations on the oxygen p-electrons together with the consideration of the broken crystal symmetry that is caused by the mixed valency lead to results that are consistent with the magnetic experiments. According to these calculations, Rb_4O_6 exhibits a highly degenerate ground state with a large number of frustrated non-collinear magnetic configurations.