MA 15: Magnetic Half-metals and Oxides I

Time: Wednesday 10:15–13:00 Location: H22

MA 15.1 Wed 10:15 H22

Quadratic MOKE studies on epitaxial $Co_2FeAl_{0.5}Si_{0.5}$ films — •Georg Wolf[1], Simon Trudel[2], Helmut Schultheiss[1], Jaroslav Hamrle[1], Koichiro Inomata[3], and Burkard Hillebrands[1] — [1]FB Physik and Landesforschungszentrum OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Department of Chemistry, University of Calgary, Canada — [3]Magnetic Materials Center, National Institute for Materials Science (NIMS), Tsukuba, Japan

Magneto-optical Kerr effect (MOKE) is often used to study the quasistatic, as well as the dynamic properties of the magnetization. While in most cases only the linear response (LMOKE) is observed, some materials show also a quadratic magneto-optical Kerr effect (QMOKE). Recently, QMOKE has been observed in the Co-based Heusler compounds [1], which are promising materials due to their predicted high spin polarization at the Fermi level.
We introduce a new MOKE setup which is designed to systematically investigate the QMOKE on Heusler thin films on a routinely basis [2]. The setup provides access to the combined LMOKE and QMOKE signal, as well as the pure QMOKE signal, each probed by an individual probing beam. We report on first results obtained on $Co_2FeAl_{0.5}Si_{0.5}$ epitaxial thin films prepared in the group of K. Inomata, Japan. The dependence of the QMOKE as a function of the annealing temperature is investigated. Financial support by the DFG Research Unit 559, New Materials with High Spin Polarization is gratefully acknowledged.
[1] O. Gaier et al. Appl. Phys. **103**, 103910 (2008).
[2] S. Trudel et al. accepted by Rev.Sci.Inst.

MA 15.2 Wed 10:30 H22

XMCD as a probe for spin-orbit interaction and spin-resolved electronic structure of Heusler compounds — •Peter Klaer[1], Michael Kallmayer[1], Elena Arbelo Jorge[1], Christian Herbort[1], Gerhard Jakob[1], Martin Jourdan[1], Christian Blum[2], Tanja Graf[2], Benjamin Balke[2], Gerhard Horst Fecher[2], Claudia Felser[2], and Hans Joachim Elmers[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, D-55128 Mainz — [2]Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg-Universität Mainz, D-55128 Mainz

To confirm theoretical predictions and optimize material properties of half-metallic Heusler alloys a characterization of the electronic structure is necessary. For this purpose x-ray magnetic circular dicroism (XMCD) is a powerful tool. In addition to the element-specific determination of the spin and orbital moment, XMCD allows a direct experimental observation of the spin-resolved unoccupied density of states (DOS) in Heusler alloys. It is shown that a substitution of Ge by Ga in alloys like Co2MnGe shifts the minority DOS maximum with respect to E_F, indicating half-metallic ferromagnetism for the whole series and satisfying the rigid-band like behavior. Results for polycrystalline bulk samples and single crystalline films are discussed. We report on the orbital to spin moment ratio versus composition, relating its variation to the symmetry of the unit cell. For the series Co2Ti1-xMnxGe the Fermi energy shifts opposite to the expected rigid band behavior, which can be explained by a charge transfer from the light 3d-element Ti with antiparallel moment to Co states.

MA 15.3 Wed 10:45 H22

The surface spin polarization of Co-based Heusler alloys — •Roman Fetzer[1], Jan-Peter Wüstenberg[1], Sabine Neuschwander[1], Martin Jourdan[2], Christian Herbort[2], Enrique Vilanova Vidal[2], Gerhard Jakob[2], Martin Aeschlimann[1], and Mirko Cinchetti[1] — [1]University of Kaiserslautern, Department of Physics and Research Center OPTIMAS, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern — [2]University of Mainz, Institute of Physics, Staudinger Weg 7, 55128 Mainz

Co-based Heusler alloys belong mainly to the family of half-metallic ferromagnets (HMFs). The predicted full spin polarization at the Fermi level due to the minority spin band gap makes this class of materials highly interesting for application in the field of spintronics. Thus, the characterization of the surface of Co-based Heusler compounds is extremely relevant for understanding and improving the performance of Heusler-based spintronics devices, like tunnel-magnetoresistance (TMR) junctions. Using Auger electron spectroscopy (AES) [1] and low energy spin polarized electron photoemission [2], we systematically studied the correlation between chemical composition and spin polarisation of the surface. For various Co-based Heusler alloys, e.g. Co_2CrAl, Co_2MnAl and $Co_2FeGa_{0.5}Ge_{0.5}$, we found different degrees of spin-polarization at the very surface region. Reasons for the distinct deviation from the predicted 100% spin polarization and the dependence on the specific surface preparation procedure will be discussed.
[1] Wüstenberg et al. , J. Phys. D: Appl. Phys. 42 (2009) 084016
[2] Cinchetti et al., J. Phys. D: Appl. Phys. 40 (2007) 1544-1547

MA 15.4 Wed 11:00 H22

Anomalous transport properties of the halfmetallic ferromagnets Co_2TiSi, Co_2TiGe, and Co_2TiSn. — •B. Balke[1], T. Graf[1], J. Barth[1], G.H. Fecher[1], A. Shkabko[2], A. Weidenkaff[2], and C. Felser[1] — [1]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, Mainz, Germany — [2]EMPA, Swiss Federal Laboratories for Materials Testing and Research, Solid State Chemistry and Catalysis, CH-8600 Duebendorf, Switzerland

This work reports on the theoretical and experimental investigations of Co_2TiZ (Z = Si, Ge, or Sn) compounds. Band structure calculations predict half-metallic ferromagnetism for all three compounds with only two bands crossing the Fermi energy in the majority channel. The magnetic moments fulfill the Slater-Pauling rule and the Curie temperatures are well above room temperature. All compounds show a metallic like resistivity for low temperatures up to their Curie temperature, above the resistivity changes to semiconducting like behavior. Additionally, we observe a large negative magnetoresistance of 55 % for Co_2TiSn at room temperature. The Seebeck coefficients are negative for all three compounds and reach their maximum values at their respective Curie temperatures and stay almost constant up to 950 K. The combination of half-metallicity and the constant large Seebeck coefficient over a wide temperature range makes these compounds interesting materials for further spincaloric investigations and thermoelectric applications. *This work is financially supported by "Stiftung Innovation Rheinland-Pfalz" and by the DfG (P1 and P7, FOR 559).*

MA 15.5 Wed 11:15 H22

Analysis of $L2_1$-ordering and study of properties on Co-based Heusler thin film samples — •Enrique Vilanova Vidal[1], Tanja Graf[2], Claudia Felser[2], and Gerhard Jakob[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz — [2]Institut für Anorganische und Analytische Chemie, Johannes Gutenberg-Universität Mainz

Heusler alloys have been intensively investigated because they are promising materials for use in spin-dependent devices. Their half-metallic properties are strongly related with the presence of $L2_1$, $B2$ and fully disordered $A2$ structure. However, a rigorous method to study the proportions of these different ordering states is still missing. Sputtered thin epitaxial $Co_2FeSi_{0.6}Al_{0.4}$, $Co_2FeGa_{0.5}Ge_{0.5}$ and Co_2MnAl films have been prepared. These films were grown on MgO (100) with and without MgO buffer layer under UHV conditions and at different substrates temperatures. The deposition procedure is discussed, and the degree of $L2_1$ order as well as transport and magnetic properties are analyzed.

MA 15.6 Wed 11:30 H22

A Fermi-level-tuned half-metallic Heusler compound: $Co_2FeAl_{0.5}Si_{0.5}$ — •Rong Shan[1,2], Hiroaki Sukegawa[1], Wenhong Wang[1], Koichiro Inomata[1], Benjamin Balke[2], Gerhard H. Fecher[2], and Claudia Felser[2] — [1]Magnetic Materials Center, National Institute for Materials Science (NIMS), 1-2-1 Sengen, Tsukuba, 305-0047, Japan — [2]Institute of Inorganic and Analytical Chemistry,Johannes Gutenberg - University, 55099 Mainz

Balke B. and Fecher G.H. et al. in our group made a theoretical prediction of Fermi level tuning in Heusler compounds, which suggested that the Fermi level of $Co_2Mn_{1-x}Fe_xSi$ and $Co_2FeAl_{1-x}Si_x$ could be tuned to achieve the half-metallicity by the element substituting easily. However, to realize this prediction is a difficulty in experiment because of the perplexing relationship between the spin polarization of the quaternary Heusler compound and its structure disorder, resulting from the thermal treatment. Very recently, we confirmed Fermi level

tuning in Heusler alloy $Co_2FeAl_{0.5}Si_{0.5}$ (CFAS). Half-metallic band gap of CFAS was proved even at room temperature by the behavior of differential conductance of CFAS/$(MgAl_2)O_x$/CoFe magnetic tunneling junctions with an unexplored crystalline $(MgAl_2)O_x$ barrier. CFAS exhibits the highest effective spin polarization (P_{eff}) at 300 K and the weakest temperature dependence of P_{eff} among all known half-metals. Further study shows that P_{eff} of CFAS decays with increasing temperature (T) following $T^{3/2}$ law perfectly, which indicates that the depolarization of CFAS is determined by spin wave excitation only.

MA 15.7 Wed 11:45 H22

Epitaxial growth of Fe_3O_4 thin films on ZnO substrates — •Andreas Müller[1], Andreas Ruff[1], Markus Paul[1], Christian Praetorius[2], Kai Fauth[2], Uwe Bauer[3], Marek Przybylski[3], Michael Sing[1], and Ralph Claessen[1] — [1]Experimentelle Physik IV, Universität Würzburg — [2]Physikalisches Institut, Universität Würzburg — [3]MPI für Mikrostrukturphysik, Halle

Magnetite (Fe_3O_4)/ zinc oxide (ZnO) heterostructures are currently explored due to their application potential in spintronics. Semimetallic Fe_3O_4 is a ferrimagnet and was predicted to possess a fully spin-polarized Fermi surface, which makes it well suited for spin injection.

We have grown Fe_3O_4 thin films epitaxially on ZnO substrates using molecular beam epitaxy. The film quality was found to be strongly dependent on the oxygen partial pressure during growth. Structural, electronic, and magnetic properties were analyzed utilizing Low Energy Electron Diffraction (LEED), HArd X-ray PhotoElectron Spectroscopy (HAXPES), Magneto Optical Kerr Effect (MOKE), and X-ray Magnetic Circular Dichroism (XMCD). Film growth on ZnO was found to be in (111) direction. HAXPES gives clear evidence for the formation of Fe_3O_4. Non-destructive depth profiling using angle dependent HAXPES measurements showed uniform growth. However, the magnetic measurements revealed reduced magnetization for films grown on ZnO.

MA 15.8 Wed 12:00 H22

Origin of Ferrimagnetism in Ti and Cr doped α-Fe_2O_3 — •Hasan Sadat Nabi and Rossitza Pentcheva — Department of Earth and Environmental Sciences, University of Munich, Theresienstr. 41, 80333 Munich, Germany

Using density functional theory (DFT) and taking into account an on-site Coulomb repulsion term (GGA+U) we perform a comparative study of Ti and Cr substitution in α-Fe_2O_3. The charge mismatch in the $FeTiO_3$-Fe_2O_3 system is identified as a driving force towards ferrimagnetism as it leads to the formation of a mixed Fe^{2+}, Fe^{3+} layer and uncompensated spins [1-2]. While a valence discontinuity is not present in the other system (Cr_2O_3-Fe_2O_3), we show that a different magnetic order and a net magnetization can be induced by controlling the concentration and arrangement of Cr ions in the Fe_2O_3-lattice, e.g. via heterostructuring. Furthermore the magnetic interaction parameters are extracted by mapping the DFT energies of different magnetic configurations to a Heisenberg Hamiltonian.

Funding by the DFG (Pe883/4-1) and ESF as well as the computational time at the Leibniz Rechenzentrum are gratefully acknowledged.
[1] R. Pentcheva and H. Sadat Nabi, Phys. Rev. B **77**, 172405 (2008).
[2] H. Sadat Nabi and R. Pentcheva, J. Appl. Phys. **105**, 053905 (2009).

MA 15.9 Wed 12:15 H22

Orbital magnetism of strongly correlated transition-metal oxides - a LSDA+DMFT study — •Gerhard Kuhn, Jan Minár, Diemo Ködderitzsch, Sergiy Mankovskyy, and Hubert Ebert — LMU München

In this study we focus on the spin-orbit coupling induced properties of strongly correlated transition-metal oxides (MnO, FeO, CoO, NiO). We used self-consistent and fully relativistic implementations of the LSDA+U and the LSDA+DMFT within the multiple scattering KKR-method. Calculations for spin and orbital magnetic moments were performed in the atomic sphere approximation and for the full potential mode. Three different magnetic structures were treated: ferromagnetic, anti-ferromagnetic 1 and anti-ferromagnetic 2. Total energies were calculated to determine the most stable magnetic structure and subsequently used to calculate the exchange-coupling constants (J_{ij}) by mapping on a Heisenberg-Model. In addition, the J_{ij}'s were calculated by the relativistic generalisation of Lichtenstein's formula and the magnetic torque method.

MA 15.10 Wed 12:30 H22

Growth and Characterisation of Mn stabilized Zirconia — •Jan Zippel, Michael Lorenz, Anette Setzer, Jörg Lenzner, Holger Hochmuth, Pablo Esquinazi, and Marius Grundmann — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik II, Linnétr. 5, 04103 Leipzig, Germany

The possibility to combine both, the electron spin as a new degree of freedom and the electron charge offers opportunities for a new generation of devices. As recently predicted [1], Mn stabilized Zirconia is proposed as a ferromagnetic semiconductor with a Curie temperature Tc above room temperature. Here we present the growth of manganese doped ZrO2 with Pulsed-Laser deposition (PLD). By introducing more than 15 at% Mn, we observe only a tetragonal or cubic crystalline structure by doing X-ray diffraction (XRD). Transmission electron microscopy (TEM), energy dispersive X-ray spectroscopy, Rutherford backscattering spectroscopy (RBS) and X-ray Photoelectron Spectroscopy (XPS) were done to check the structural properties as well as the Mn content and the stoichiometry. Beside the structural also the electronic and magnetic properties were investigated. We compare the conductivity of pure ZrO2 either with Mn doped ZrO2 or with Mn stabilized Zirconia (MnSZ) co-doped with Al, Y, and Nb. Superconducting quantum interference device (SQUID) measurements revealing a superparamagnetic behavior at low temperatures (T = 5K) but, up to now, no room temperature ferromagnetism.

[1] S. Ostanin et al., Phys. Rev. Lett 98, 0161011 (2007).

MA 15.11 Wed 12:45 H22

Correlation between Curie temperature and carrier density of electron-doped EuO - is there an intrinsic limit on T_C? — •Thomas Mairoser[1], Andreas Schmehl[1], Jochen Mannhart[1], Alexander Melville[2], Tassilo Heeg[2], Darrell G. Schlom[2], Peter Böni[3], Lea Canella[3], and Jürgen Schubert[4] — [1]Universität Augsburg — [2]Cornell University, USA — [3]Technische Universität München — [4]Forschungszentrum Jülich

The ferromagnetic semiconductor europium oxide exhibits a multitude of giant properties, such as metal-to-insulator transitions, a colossal magneto-resistance, and very pronounced magneto-optic effects. The recently demonstrated spin-polarization of $> 90\,\%$ in the ferromagnetic state [A. Schmehl *et al.*, Nat. Mat. **6**, 882 (2007)] and its excellent electronic compatibility with Si make it an interesting candidate for semiconductor based spintronics. Nevertheless the low Curie temperature (T_C) of 69 K of undoped EuO is a major obstacle for the use of this outstanding material in commercial spintronic applications.

By electron doping EuO with donor impurities, T_C can substantially be increased exploiting an additional exchange interaction that is mediated via the conduction electrons.

Here we report on measurements of T_C and the carrier densities by Hall effect on La and Gd doped EuO films grown over a wide range of doping concentrations and growth conditions. The experiments show that only a small fraction of the introduced impurities actually act as donors even for optimized growth parameters. Furthermore we found a strong correlation between Curie temperatures and carrier densities.