MA 3: Magnetic Heuslers, Half-metals and Oxides (jointly with TT)

Time: Monday 9:30–12:45 Location: H 0112

MA 3.1 Mon 9:30 H 0112

Half-metallic compensated ferrimagnetic behaviour of $Mn_{1.5}V_{0.5}$FeAl Heusler compound — •Rolf Stinshoff, Peter Adler, Gerhard Fecher, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Half-metals, i.e. materials exhibiting 100 % spin polarization, naturally attract much interest in spintronics [1]. Some of them have already shown their potential in applications such as magnetic tunneling junctions. Despite the very high TMR ratios achieved at low temperatures using half-metallic materials, further technological requirements, such as low stray fields, temperature stability etc., still have to be improved. In this context, some advantages are provided by the group of completely compensated ferrimagnets which still keep the half-metallicity. Several of them were predicted theoretically within the Heusler family. Here we will discuss the experimentally measured characteristics (structural, magnetic and transport properties) of the newly synthesized $Mn_{1.5}V_{0.5}$FeAl Heusler material, which is suggested to be a fully compensated half-metallic ferromagnet by the first principle calculations [2].

[1] R. A. de Groot, F. M. Müller, P. G. van Engen, K. H. J. Buschow, Phys. Rev. Lett. **50**, 2024-2027 (1983)

[2] S. Wurmehl, H. C. Kandpal, G. H. Fecher, C. Felser, J. Phys. Condens. Matter **18**, 6171-6181 (2006)

MA 3.2 Mon 9:45 H 0112

High-throughput screening for antiferromagnetic Heusler compounds using density functional theory — •Jan Balluff, Markus Meinert, and Günter Reiss — Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Germany

Due to the exchange bias effect, antiferromagnetic compounds are of particular interest for the field of spintronics. Since Heusler compounds are a very versatile family of alloys, we attempt to find promising antiferromagnetic compounds unknown by now. We report on a high-throughput screening among the Heusler compounds for stable antiferromagnetic systems. Starting from a detailed evaluation of raw magnetic data for Heusler compounds extracted from the AFLOWLib [1], we extend the data by explicitly checking for stable antiferromagnetic ground states. [1] S. Curtarolo et al., Comp. Mat. Sci. 58 , 218 (2012)

MA 3.3 Mon 10:00 H 0112

Spin-selective electron localization induced by disorder in Mn-Co-Al Heusler alloys — •Sunil Wilfred D'Souza, Siham Ouardi, Lukas Wollmann, Stanislav Chadov, and Claudia Felser — Max-Planck-Institut für Chemische Physik fester Stoffe

Understanding the role of disorder opens new alternatives in the state-of-the-art design of the multicomponent materials. First proposals to improve the electron transport characteristics by constructive chemical disorder were already suggested for the tetragonal non-halfmetallic ferrimagnetic Mn_3Ga-based Heusler alloys, where the possibility of the spin-selective electron localization was demonstrated by the first-principles. Here we consider the spin-selective electron localization within the cubic $Mn_{2-x}Co_{1+x}Al$ ($0 \leq x \leq 1$) Heusler series. In contrast to the strongly anisotropic tetragonal case, the isotropic cubic geometry allows for an easier experimental check of the proposed spin-selective electron localization. The residual transport properties, i.e. spin-projected resistivities were calculated within the Kubo-Greenwood linear response formalism, using Coherent Potential Approximation (CPA) description for the electron localization, within the framework of the fully-relativistic SPR-KKR Green's function method. Here we also give the comparison with the first experimental data.

MA 3.4 Mon 10:15 H 0112

Advantages of constructive disorder: design of the spin-selective electron localization in Mn_3Ga-derivatives — •Stanislav Chadov, Sunil Wilfred D'Souza, Lukas Wollmann, and Claudia Felser — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

Understanding the role of disorder opens new alternatives in the state-of-the-art design of the multicomponent materials. Theoretically we will try to design a situation in which the constructive disorder serves as a mechanism preventing the propagation of certain quasiparticles, namely the spin-down electrons – the so-called *spin-selective* electron localization. Here we make use of chemical disorder induced by the small stoichiometric variations. As a suitable example, we take a non-halfmetallic Mn_3Ga Heusler, and subsequently develop the appropriate constructive disorder scheme justifyed by the first-principles calculations based on the Coherent Potential Approximation (CPA) and Kubo-Greenwood linear response formalsim within the framework of the SPR-KKR Green's function method. As it follows from our results, almost any relatively small substitution of Mn by other $3d$ transition element (except of Cu) leads to a dramatic increase of the spin-polarization along the tetragonal crystalline axis.

MA 3.5 Mon 10:30 H 0112

Superconducting TiN seed layer for Heusler compounds — •Alessia Niesen[1], Manuel Glas[1], Daniel Ebke[2], Jan Schmalhorst[1], and Günter Reiss[1] — [1]Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Germany — [2]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany

TiN thin films were prepared by DC and RF magnetron sputtering in an UHV sputtering system. Epitaxial growth was achieved on MgO (001) and $SrTiO_3$ (001) substrates at deposition temperatures above 450°C. The crystallographic and surface properties of TiN were determined by X-ray diffraction (XRD) and reflection (XRR) measurements. In addition, atomic force microskopy (AFM) was performed to verify the low roughness ($< 1\,nm$) measured by the XRR. The out-of-plane lattice constant and the resistivity of TiN reached the theoretical predicted values of 4.24 Å and nearly $20\,\mu\Omega cm$ (bulk value). 4-terminal transport measurements in a closed cycled helium cryostat showed a phase transition to the superconducting state at temperatures below 5 K for TiN deposited at 450°C on MgO and $SrTiO_3$ substrate. The suitability of TiN as seed layer for ferromagnetic materials like Iron and Heusler compounds, e. g. Co_2FeAl and $Mn_{3-x}Ga$, was investigated by analysing the crystallographic and magnetic properties. Epitaxial growth of both Heusler compounds (Co_2FeAl and $Mn_{3-x}Ga$) on a TiN seed layer has been proven for various deposition temperatures. Hall-measurements additionally showed a higher coercitivity and squareness ratio for Mn-Ga thin films when prepared on a TiN buffer.

MA 3.6 Mon 10:45 H 0112

Mn-based candidates for rare earth free permanent magnet — •Adel Kalache, Bayardulam Jamiyansuren, Siham Ouardi, Guido Kreiner, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Permanent magnets are used in a wide range of applications from hybrid cars and wind turbines to computer hard-disk drives. Rare earth (RE) magnets such as Nd-Fe-B and Sm-Co show unique hard magnetic performance but are subject to both price and supply issues. New RE free permanent magnets are also needed to fill the gap between the low cost hexagonal ferrites and the expensive RE magnets. Some Mn-based intermetallic compounds are promising candidates because of their high Curie temperature and their tetragonal structure of the $L1_0$ type or distorted Heusler $D0_{22}$ type. The resulting intrinsic uniaxial magnetic anisotropy leads to appreciable hard magnetic properties. The synthesis of Mn-based RE free magnets with melt spinning technique improves some extrinsic properties such as microstructure and grain size. These features allow an increase of the coercivity of material, leading to higher figure of merit BH_{max}. Structural characterization and magnetic properties of some tetragonal Mn-based compounds such as Mn-Ga and Mn-Ge will be presented. Neutron diffraction is reported for $Mn_{60}Ga_{40}$. Substitution of Mn with other transition metals will also be discussed in order to improve the magnetic hardness.

15 min. break

MA 3.7 Mon 11:15 H 0112

Calculation of electronic structure and field-induced magnetic collapse in ferroic materials — •Peter Entel — Faculty

of Physics, University Duisburg-Essen, D-47048 Duisburg, Germany

We have performed ab initio electronic structure calculations and Monte Carlo simulations of Fe-Rh, Mn-Ga-C and Heusler intermetallics alloys such as Ni-Co-Cr-Mn-(Ga, In, Sn) which are of interest for magnetic shape-memory devices, solid-state refrigeration and energy systems, an emerging technology involving solid systems. The calculations reveal that the important magnetic phase diagrams of these alloys which show the magnetic collapse and allow predictions of the related magnetocaloric effect which they exhibit at finite temperatures, can be obtained by the ab initio computations alone. This is a one-step procedure from theory to alloy desigan of ferroic functional devices.

MA 3.8 Mon 11:30 H 0112

Ab initio study of tetragonal Heusler alloys for magnetic applications with high anisotropies — •Heike C. Herper, Yaroslav O. Kvashnin, and Olle Eriksson — Department of Physics and Astronomy, Uppsala University, Sweden

Materials with high magnetic anisotropy (MAE) are of broad technological interest whereby typical magnets with high MAE are based on expensive materials such as Pt or Nd. Therefore, cheap and abundant replacements are demanded. Heusler alloys are of special interest because their magnetic and structural properties can be quite easily designed by composition. Here we present an ab initio study for a series of tetragonal Ni-based Heusler alloys Ni_2YZ with (Y = Mn, Fe, Co) and Z varying from B to Sn. Combined VASP and RSPt investigations reveal MAE values for $L2_1$ ordered Co containing alloys which are comparable to the Mn-Ga based alloys found in literature. However, for e/a values larger than 32 they tend to inverse order which is accompanied by a significant reduction of the MAE. Even though the MAE values for alloys with Y = Fe are found to be smaller compared to the Ni_2CoZ alloys, the maximum energy products are similar. In contrast to the $L2_1$ ordered Ni_2CoZ systems out of plane MAE has been observed for several Ni_2FeZ alloys.

MA 3.9 Mon 11:45 H 0112

Magnetism in tetragonal Heusler compounds — •Lukas Wollmann[1], Stanislav Chadov[1], Jürgen Kübler[2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany. — [2]Institut für Festkörperphysik, Technische Universität Darmstadt, Darmstadt, Germany

Compounds with uniaxial anisotropy are of general interest in the field of magnetism, and in particular within the emerging field of spintronics. Uniaxial anisotropy is an inherent property of many tetragonal Heusler compounds. Here we report on a comprehensive study on tetragonal Manganese-based Heusler compounds, by starting from a set of cubic parent systems and continuing with the mechanisms of their tetragonal distortion, in particular focusing on the magnetic properties, and explaining the microscopic origin of the observed properties, as for example, for the magnetocrystalline anisotropy. Rather high anisotropy values were obtained for those systems containing heavy transition metals, which suggests them as candidate materials for spin transfer torque magnetization switching applications.

MA 3.10 Mon 12:00 H 0112

Phase separation in NiSn- and CoSb-based Half-Hesleur alloys — Joaquin Miranda Mena, •Heiko G. Schoberth, Thomas Gruhn, and Heike Emmerich — Material- und Prozesssimulation, Bayreuth University. Universitätsstraße 30 D-95448 Bayreuth, Germany

We combine DFT calculations, Monte Carlo simulations and mean field models to study the thermodynamic conditions for phase separation in two families of quaternary-Half-Heusler alloys. In the first family, γNiSn (γ =TiHf, TiZr), we found that phase separation is achieved in the range 500-700 K, but no phase separation is present when alloying with γ=ZrHf. For CoTi(1-x)ZxSb (Z=Sc, Cr, Mn, Fe, Cu) we found transition temperatures in the range 800-3000 K. The transition temperature is favored at nearly one third of concentration (x). However, at large x some materials do not present phase separation, but rather a type of crystal order. We discuss these results in the view of thermoelectrics, where apparently induced phase separation enhances the figure of merit.

MA 3.11 Mon 12:15 H 0112

Highest Curie temperature in Co-Fe based Heusler compounds — •Julia Erika Fischer[1], Siham Ouardi[1], Gerhard Fecher[1], Guido Kreiner[1], Peter Adler[1], Claudia Felser[1], Simone Fabbrici[2], and Franca Albertini[2] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Institute of Materials for Electronics and Magnetism CNR, Parma, Italy

Half-metallic ferromagnetic Co-based Heusler compounds are one of the most promising class of materials for high performance spintronic devices due to the recently experimentally demonstrated strong spin polarization and their reported high Curie temperatures [1, 2].
We have prepared a series of polycrystalline Co-Fe based Heusler alloys and studied the structural and magnetic properties. From thermomagnetic analysis measurements we found Curie temperatures of more than 1200 K, which are the highest values in Heusler alloys so far. Therefore, a higher thermal stability of magnetization is expected even for moderate device temperatures. In particular, the Co-Fe disorder was investigated by Mößbauer spectroscopy to study the influence on the magnetic properties.

[1] B. Balke et al., Sci. *Technol. Adv. Mater.* 9, 014102 (2008).
[2] M. Jourdan et al., *Nat. Commun.*, 5 (3974), 1 (2014).

MA 3.12 Mon 12:30 H 0112

Antiferromagnetic order in CuMnSb crystal and its stability — •Frantisek Maca, Vaclav Drchal, and Josef Kudrnovsky — Institute of Physics ASCR, Praha, Czech Republic

It is well known that the ground state of the CuMnSb is antiferromagnetic with alternating ferromagnetic layers in the <111> direction - the AFM(111) structure. The first ab initio calculations comparing nonmagnetic, ferromagnetic and AFM(111) structures [1] also have shown that the antiferromagnetic state has the lowest total energy. However, we found by using FLAPW and TB-LMTO calculations that the ideal AFM(001) structure has always lower total energy than the AF(111).

Experimental measurements show a high resistivity of CuMnSb samples which indicates the presence of disordered impurities. We compare formation energies for various defects in order to find the type of disorder which favors the AFM arrangement. Calculations indicate as the most probable candidate the Mn-Cu swapping. We show that presence of disorder and electron correlations are needed for realistic theoretical description. The total energy results are supported by discussion of magnetic exchange interactions.

[1] T. Jeong, Ruben Weht, and W. E. Pickett, Phys. Rev. B 71, 184103 (2005).