MA 35: Magnetic Heusler Compounds I

Time: Wednesday 15:00–18:00 Location: H 0112

Topical Talk MA 35.1 Wed 15:00 H 0112

Heusler compounds: theory and experiments on their electronic structure. — •G. H. Fecher — Max Planck Institute for Chemical Physics of Solids, Dresden

It is well known that Heusler compounds are famous for the occurrence of half-metallic ferromagnetism. Recently they were also suggested to belong to the group of topological insulators. It will be shown that there are some more interesting features in the electronic structure of Heusler compounds between metals and insulators and how they can be designed to exhibit spin gapless semiconductivity and spin gapless antiferromagnetism. Spin gapless semiconductors and halfmetallic antiferromagnets are classes of materials that bridge the gap between the properties of metals and semiconductors. Both exhibit peculiar halfmetallic transport properties and are closely related to halfmetallic ferromagnets. In halfmetallic materials, transport is mediated by electrons having only one kind of spin, i.e., the minority or the majority spin. Spin gapless semiconductors exhibit an additional phenomenon, namely, an open bandgap in one spin channel and a closed bandgap (zero bandgap) in the other. Further, halfmetallic antiferromagnets, also referred to as halfmetallic completely compensated ferrimagnets, exhibit spin order without any macroscopic magnetization. They become spin gapless antiferromagnets when the conducting spin channel exhibits a zero bandgap. The evidence for these phenomena will be exemplified by comparing ab-initio calculations to measurements of the electronic structure by photoemission and electronic transport properties.

MA 35.2 Wed 15:30 H 0112

***Ab initio* investigation of $Co_2FeSi_{1-x}Z_x$ and $Co_2Fe_{1-x}Z_{1+x}$ Heusler alloys: Magnetism and tetragonal instability** — •Heike C. Herper and Peter Entel — Faculty of Physics and CeNIDE, University of Duisburg-Essen, 47048 Duisburg, Germany

Since the magnetic properties of Heusler compounds can be relatively easily controlled by composition these alloys seem to be suitable for different magnetic applications, e.g., in magnetoelectronic and magnetocaloric devices and one can think of multifunctional devices. Here, we present an *ab initio* study of $Co_2FeSi_{1-x}Z_x$ and $Co_2Fe_{1-x}Z_{1+x}$ Heusler alloys with Z = Al, Sb, Sn. Electronic properties have been studied within the density functional theory using the VASP and SPRKKR code. Information about finite temperature properties is obtained from Monte Carlo simulations of the classical Heisenberg model with *ab initio* determined exchange coupling constants.

We have investigated the composition dependence of the magnetic transition temperatures and the spin polarization which are important for spintronic applications as well as the tendencies of martensitic phase transformation. Replacing Si in Co_2FeSi partially by Fe the cubic phase is preferred and spin polarization remains large, whereas, Si excess stabilizes the tetragonal phase, but spin polarization is drastically reduced. However, if fractions of Si are replaced by Sb the system also exhibits a tetragonal instability, but with reasonable large spin polarization.

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MA 35.3 Wed 15:45 H 0112

Optical properties of Co_2FeZ half-metallic Heusler compounds — •Jaroslav Hamrle[1], Dominik Legut[1], Kamil Postava[1], Jaromír Pištora[1], Enrique Vilanova[2], Mirko Emmel[2], and Gerhard Jakob[2] — [1]Department of Physics and Nanotechnology Centre, VSB - Technical University of Ostrava, Czech Republic — [2]Institute of Physics, Mainz University, Germany

Common materials for plasmonic applications are gold and silver, as they provide low damping and negative value of real part of the permittivity. Nowadays, there is a need of new materials, which can provide both plasmonic excitations and magneto-optical activity. Co_2-based half metallic Heusler compounds are promising materials for this purpose, as there are several similarities in electronic band structure for exited states between gold, silver and the majority band of Co_2-based Heusler compounds for photon energies smaller than minority electron gap size (i.e. below 1 eV).

Within this contribution we present complex refractivity index, determined in range from mid-infrared (mid-IR) to near-ultraviolet, of half-metallic Heusler compounds Co_2FeSi, $Co_2FeAl_{0.4}Si_{0.6}$ and $Co_2FeGa_{0.5}Ge_{0.5}$ measured by ellipsometry and IR reflectometry. The optical spectra were computed in the single electron picture within the framework of the DFT. The interband as well as intraband transitions were considered.

MA 35.4 Wed 16:00 H 0112

Electronic, structural, and magnetic properties of the half-metallic ferromagnetic quaternary Heusler compounds CoFeMnZ (Z = Al, Ga, Si, Ge) — •Vajiheh Alijani, Juergen Winterlik, Gerhard Fecher, and Claudia Felser — Institute for Inorganic and analytical Chemistry, Johannes Gutenberg University, 55099 Mainz, Germany

Half-metallic ferromagnets exhibit 100% spin polarization at the Fermi energy and therefore are ideal candidates for spin-injection devices. Several materials besides Heusler compounds have been predicted to exhibit half-metallicity. Several quaternary-or pseudo-ternary Heusler compounds have been designed in order to tailor the middle of the gap exactly to the Fermi energy. For symmetry reasons (T_d), quaternary Heusler compounds with a 1:1:1:1 stoichiometry are substantially different from the $L2_1$ pseudo-ternary Heusler compounds with O_h symmetry and $2:[(1-x):x]:1$ or $2:1:[(1-y):y]$ stoichiometry.

The quaternary intermetallic Heusler compounds CoFeMnZ (Z = Al, Ga, Si, Ge) with 1:1:1:1 stoichiometry were predicted to exhibit half-metallic ferromagnetism by ab-initio electronic structure calculations. The compounds were synthesized using an arc-melting technique and the crystal structures were analyzed using X-ray powder diffraction. The electronic properties were investigated using HAXPES. The low-temperature magnetic moments, as determined from magnetization measurements, follow the Slater-Pauling rule, confirming the proposed high spin-polarizations. All compounds have high Curie-temperatures, allowing for applications at room temperature and above.

MA 35.5 Wed 16:15 H 0112

Curie temperatures of Mn_2CoZ inverse Heusler compounds — •Markus Meinert, Jan Schmalhorst, and Günter Reiss — Dünne Schichten und Physik der Nanostrukturen, Fakultät für Physik, Universität Bielefeld, 33501 Bielefeld

The exchange interactions and Curie temperatures of inverse Heusler compounds Mn_2CoZ (Z = Al, Ga, In, Si, Ge, Sn, Sb) with the Hg_2CuTi structure have been studied by density functional theory. Due to the direct Mn-Mn exchange interaction in Mn_2CoZ, the Curie temperature *decreases*, although the total moment *increases* when the Z valence electron number is increased. The coupling between the nearest-neighbor Mn atoms scales with the magnetic moment of the Mn atom on the C site. A negative pressure dependence of the Curie temperature is predicted, which follows from decreasing magnetic moments under pressure. Curie temperatures of more than 800 K are predicted for Mn_2CoAl (890 K), Mn_2CoGa (886 K), and Mn_2CoIn (845 K), which are in reasonable agreement with experiments.

15 min. break

MA 35.6 Wed 16:45 H 0112

Pressure dependence of Curie temperature and resistivity of complex Heusler alloys — •Vaclav Drchal[1], Shyamal Bose[2], Josef Kudrnovsky[1], and Ilja Turek[3] — [1]Institute of Physiscs AS CR, Praha, Czech Republic — [2]Brock University, St. Catharines, Canada — [3]Institute of Physics of Materials, AS CR, Brno, Czech Republic

Using first-principles electronic structure methods, we have calculated the Curie temperature and resistivity of random quaternary Heusler alloys $(Ni_{1-x}Pd_x)_2MnSn$ and $(Ni_{1-x}Cu_x)_2MnSn$ [1] and studied their dependence on the external hydrostatic pressure [2]. The Curie temperatures were calculated within the random-phase approximation applied to the Heisenberg Hamiltonian, whose parameters were determined using the density functional theory. The Curie temperature increases with pressure in $(Ni_{1-x}Pd_x)_2MnSn$ alloys for all concentrations x while the crossover from the increase to the decrease of the Curie temperature with pressure takes place for $x > 0.7$ in $(Ni_{1-x}Cu_x)_2MnSn$ Heusler alloys. The spin-disorder induced part of the resistivity in $(Ni_{1-x}Pd_x)_2MnSn$ Heusler alloys, calculated by using

the disordered local moment model, is presented. Finally, we discuss qualitatively the results on the basis of Anderson's superexchange and Stearn's model of the indirect exchange between localized and itinerant d-electrons.

[1] S.K. Bose et al.: Phys. Rev. B **82** 174402 (2010). [2] S.K. Bose et al.: Phys. Rev. B **84** 174442 (2011).

MA 35.7 Wed 17:00 H 0112

Structural and magnetic properties of $Mn_2Rh_{1-x}Co_xSn$ and $Mn_{2+x}Rh_{1-x}Sn$ Heusler alloys — •Olga Meshcheriakova[1], Juergen Winterlik[1], Gerhard Fecher[1,2], and Claudia Felser[1,2] — [1]Institute for Inorganic and Analytical Chemistry, Johannes Gutenberg - University, Mainz — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Mn_2-based Heusler compounds are promising candidates for spintronic applications as they are known to crystallize with cubic and tetragonal structures or exhibit cubic-tetragonal phase transitions. Sn-containing compounds have only a small lattice mismatch with MgO thus providing higher symmetry correlation between magnetic film and tunneling barrier. Quaternary $Mn_2Rh_{1-x}Co_xSn$ and $Mn_{2+x}Rh_{1-x}Sn$ Heusler alloys have been synthesized with a step of $x = 0.1$ and their magnetic properties were experimentally investigated. In the present work the structural and magnetic properties are discussed depending on the Rh and Co content. The first series undergoes a cubic-tetragonal transition at $x = 0.5$, while the latter one experiences a hexagonal-tetragonal change of structure. The presence of Co increases the Curie temperature keeping the magnetic moment unchanged.

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MA 35.8 Wed 17:15 H 0112

Electronic properties of $Co_2Fe_xMn_{1-x}Si$ Heusler alloys studied by hard X-ray photoelectron spectroscopy. — •A. Gloskovskii[1], S. Thiess[3], S. Ouardi[1], G. H. Fecher[1,2], W. Drube[3], B. Detlefs[4], T. Kubota[5], Y. Ando[5], and C. Felser[1,2] — [1]Institute of Inorganic Chemistry and Analytical Chemistry, JoGu University, Mainz — [2]Max Planck Institute for Chemical Physics of Solids, Dresden — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg — [4]ESRF, Grenoble — [5]Department of Applied Physics, Graduate School of Engineering, Tohoku University, Sendai

Fully epitaxial magnetic tunnel junctions (MTJs) with a Co_2YZ thin film as a base electrode and a MgO tunnel barrier exhibit high TMR ratios. Quaternary $Co_2Fe_xMn_{1-x}Si$ (CFMS) Heusler alloys are even more promising because the substitution of Mn by Fe increases the number of valence electrons and therefore leads to higher Curie temperatures above 1000 K. The maximum TMR ratio for CFMS-CoFe MTJs was found for Fe fractions of between x=0.4 and 0.6. Half-metallicity disappears for the samples with x$\geq$0.8.

A $B2$ and $L2_1$ site ordered stack of MgO substrate/ Cr [40 nm] buffer layer/$Co_2Fe_xMn_{1-x}Si$ [30 nm]/MgO[2 nm]/AlO_x [1.3 nm] (x = 0, 0.2 ... 1.0) films was studied at beamline P09 at PETRA III and beamline ID32 at the ESRF. The hard X-Ray photoelectron spectroscopy (HAXPES) studies were performed with an excitation energy of 6 keV. It was found that the position of Co 2p core levels and the density of states in the valence band region strongly depend on the Fe/Mn ratio.

MA 35.9 Wed 17:30 H 0112

Symmetry of valence states of Heusler compounds explored by linear dichroism in hard X-ray photoelectron spectroscopy — •S. Ouardi[1], G. H. Fecher[1,2], C. Shekhar[2], B. Balke[1], A. Gloskovskii[1], C. Felser[1,2], E. Ikenaga[3], S. Ueda[4], and K. Kobayashi[4] — [1]Institute of Inorganic Chemistry and Analytical Chemistry, Johannes Gutenberg - University, Mainz — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany. — [3]Japan Synchrotron Radiation Research Institute, SPring-8, Hyogo, Japan — [4]National Institute for Materials Science, SPring-8, Hyogo, Japan

In the present work, a combination of the the linear dichroism in the angular distribution (LDAD) with the bulk-sensitive hard-x-ray photoelectron spectroscopy (HAXPES) technique was used to investigate the symmetry of the valence states of magnetic, semiconducting and gapless Heusler compounds with $C1_b$ structure. High-resolution photoelectron spectroscopy was performed with an excitation energy of $h\nu = 7.938$ keV. The linear polarization of the photons was changed using an in-vacuum diamond phase retarder. The valence band spectra exhibit the typical structure expected from first-principles calculations of the electronic structure of these compounds. Noticeable linear dichroism is found in the valence band of the materials and this allows for a symmetry analysis of the contributing states. The differences in the spectra are found to be caused by symmetry-dependent angular asymmetry parameters, and these occur even in polycrystalline samples without preferential crystallographic orientation.

MA 35.10 Wed 17:45 H 0112

Elastic properties and stability of tetragonal Heusler compound — •S. S. Naghavi[1], S.-C. Wu[1,2], G. H. Fecher[1,2], and C. Felser[1,2] — [1]Institute for Inorganic and Analytical Chemistry, Johannes Gutenberg - University, Mainz — [2]Max Planck Institute for Chemical Physics of Solids, Dresden

Cubic-tetragonal phase transition in the Heusler compounds is of particular interest because tetragonally distorted Heusler compounds with a magnetic anisotropy in the perpendicular axis are promising for spin-torque applications. Therefore, theoretical prediction of new tetragonal Heusler compounds is quiet important and also challenging. A different approach to analyze the structural phase transition is to consider the mechanical instability of the stressed lattice, which is a reliable method for a perfect crystal at the zero applied stress. Rather than mechanical instability, determination of elastic constants gives valuable information about the type of bonding, hardness, velocity of sound, Debye temperature, etc. To calculate the elastic constants and related properties highly accurate, one needs an accurate DFT calculator. Therefore, we used FP-LAPW implemented in the Wien2K to calculate the elastic constants of tetragonally distorted structures. This method together with GGA(PPE) exchange-correlation functionals ensure a reliable estimation for electronic structure calculations of Heusler compounds. It is shown that the calculated elastic constants provide a correct estimation for the study of phase transition in the Heusler compounds.