MA 8: Magnetic Materials II

Time: Monday 15:15–17:15 Location: H22

MA 8.1 Mon 15:15 H22

New half-metallic ground state in non-ideal $Co_{2-x}Mn_{1+x}Si$ — •Björn Hülsen[1], Peter Kratzer[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin — [2]Fachbereich Pysik, Universität Duisburg-Essen, Lotharstr. 1, D-47048 Duisburg

The half-metallic full Heusler alloy Co_2MnSi is a promising candidate for spintronics applications. Heterostructures like magnetic tunnel junctions where Co_2MnSi is incorporated with metal oxide layers are annealed with temperatures of $400 - 500°C$ during the growth process. To access the finite-temperature properties of Co_2MnSi we apply a combined approach of density functional theory (DFT), cluster expansion (CE), and Monte Carlo (MC) techniques. Since the most abundant defects in Co_2MnSi are Mn and Co antisites which are also the ones that influence the electronic structure most significantly, we regard Co_2MnSi as a pseudo-binary alloy and perform a CE that takes only the interactions between the Co and Mn atoms into account, while the Si atoms are confined to their sublattice. The coefficients of this CE are fitted to the energies of 59 structures that have been determined by DFT calculations using the full-potential linearized augmented plane wave method. Two of the seven predicted ground states show a spin gap, one is the well known $L2_1$ structure while the new half-metallic ground state has a Mn concentration of 50%. The effective Hamiltonian is used as input for a simulated annealing of ideal and non-ideal compositions of $Co_{2-x}Mn_{1+x}Si$ that allow the computation of the equilibrium configurations of these structures.

MA 8.2 Mon 15:30 H22

GdPdSb as a weak ferromagnet and half metal at low temperature — •Frederick Casper, Hem Kandpal, and Claudia Felser — Institut für Analyt. Chemie und Anorg. Chemie, Johannes Gutenberg Universität Mainz, Staudinger Weg 9, D-55099 Mainz, Germany

REPdSb compounds exhibit a variety of interesting properties, such as Kondo effect, half metallic behaviour and heavy fermion behaviour with magnetic instability [1]. GdPdSb crystallizes in the LiGaGe structure (space group P 6_3 m c). The self-consistent band structure calculations using the full potential linear augmented plane wave (FLAPW) method [2] confirmed the antiferromagnetic behaviour of this compound with $T_N = 14K$ [3].

The antiferromagnetic configuration is more stable compared with the ferromagnetic configuration, but the energy difference is very small between antiferromagnetic and ferromagnetic configuration; therefore one could expect (weak) ferromagnetic behaviour at low temperature. SQUID measurements show a rising of the magnetic susceptibility below T_N at 7K. Also a small hysteresis loop is observed. This could be of possible weak ferromagnetic ordering in agreement with the prediction of the calculation. According to band structure calculations, ferromagnetic ordered GdPdSb is half metallic, which is the first half metallic ferromagnet with LiGaGe structure.

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MA 8.3 Mon 15:45 H22

X-ray diffraction and quadratic MOKE-measurements on Co_2MnSi-alloys — •Sebastian Hermsdörfer[1], Oksana Gaier[1], Yuya Sakuraba[2], Jaroslav Hamrle[1], Yasuo Ando[2], Burkard Hillebrands[1], and Terunobu Miyazaki[2] — [1]Fachbereich Physik und Forschungsschwerpunkt MINAS, Technische Universität Kaiserslautern, Erwin-Schrödinger-Str. 56, 67661 Kaiserslautern, Germany — [2]Department of Applied Physics, Graduate School of Engineering, Tohoku University, Aoba-yama 6-6-05, Aramaki, Aoba-ku, Sendai 980-8579, Japan

Heusler alloys are attracting more and more attention due to their theoretical spin polarization of up to 100 % at the Fermi level. The full Heusler alloy Co_2MnSi should have a theoretical spin polarization of 100 % in its $L2_1$-structure whereas the spin polarization should be lower for the B2-structure.

In this talk, the influence of the B2 to $L2_1$ transition on the magnetic properties of the Heusler alloy Co_2MnSi is reported. The transition from one structure to the other is obtained by different post-growth annealing temperatures. The crystal structure itself was determined by X-ray diffraction measurements and shows the transition between the two ordered states. Quadratic MOKE measurements have been carried out for studying the magnetic properties and show a distortion of the cubic crystal structure in the transition phase.

The work was supported by the Research Unit 559 "New materials with high spin polarization" funded by the Deutsche Forschungsgemeinschaft and by the NEDO Grant.

MA 8.4 Mon 16:00 H22

Influence of the B2 to $L2_1$ phase transition on exchange interaction and coercive field in the Co_2MnSi Heusler compound — •Oksana Gaier[1], Jaroslav Hamrle[1], Sebastian Hermsdörfer[1], Burkard Hillebrands[1], Yuya Sakuraba[2], and Yasuo Ando[2] — [1]Fachbereich Physik and Forschungsschwerpunkt MINAS, Technische Universität Kaiserslautern, Erwin-Schrödinger-Straße 56, 67663 Kaiserslautern, Germany — [2]Department of Applied Physics, Graduate School of Engineering, Tohoku University, Aoba-yama 6-6-05, Aramaki, Aoba-ku, Sendai 980-8579, Japan

It has been shown theoretically that the spin polarization of the Heusler compound Co_2MnSi is very sensitive to the atomic disorder in the crystal lattice. We have investigated the influence of the disorder between Mn and Si sites on the magnetic properties of thin epitaxial Co_2MnSi films with crystal structures varying from B2 to $L2_1$ phases. The phase transition between B2 and $L2_1$ was obtained by different annealing temperatures of the sample after its deposition. Brillouin light scattering studies show very small changes of the exchange stiffness constant and the saturation magnetization upon the B2 to $L2_1$ phase transition. On the other hand, magneto-optical magnetometry reveals that the anisotropy energy gradually decreases when the crystal structure changes from B2 to $L2_1$.

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MA 8.5 Mon 16:15 H22

Electronic structure, magnetism, and disorder in the Heusler compound Co_2TiSn — •Hem Chandra Kandpal[1], Vadim Ksenofontov[1], Marek Wojcik[2], Ram Seshadri[3], and Claudia Felser[1] — [1]Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg-Universität, Staudinger Weg 9, 55099 Mainz, Germany — [2]Institute of Physics, Polish Academy of Sciences, Al. Lotnikow 32/46, 02-668 Warszawa, Poland — [3]Materials Department and Materials Research Laboratory, University of California, Santa Barbara, CA 93106, USA

Polycrystalline samples of the Heusler compound Co_2TiSn have been prepared and studied using bulk techniques (X-ray diffraction and magnetization) as well as local probes (^{119}Sn Mössbauer spectroscopy and ^{59}Co nuclear magnetic resonance spectroscopy) in order to determine how disorder affects half-metallic behavior and also, to establish the joint use of Mössbauer and NMR spectroscopies as a quantitative probe of local atom ordering in these compounds. Additionally, density functional electronic structure calculations on ordered and partially disordered Co_2TiSn compounds have been carried out at a number of different levels of theory in order to simultaneously understand how the particular choice of DFT scheme as well as disorder affect the computed magnetization. Our studies suggest that a sample which seems well-ordered by X-ray diffraction and magnetization measurements can possess up to 10% of antisite (Co/Ti) disordering. Computations similarly suggest that even 12.5% antisite Co/Ti disorder does not destroy the half-metallic character of this material.

MA 8.6 Mon 16:30 H22

Mössbauer and NMR study of Heusler alloy $Co_2Mn_{1-x}Fe_xSi$ — •Vadim Ksenofontov[1], Hem Chandra Kandpal[1], Marek Wojcik[2], Benjamin Balke[1], and Claudia Felser[1] — [1]Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg-Universität, Staudinger Weg 9, 55099 Mainz, Germany — [2]Institute of Physics, Polish Academy of Sciences, Al. Lotnikow 32/46, 02-668 Warszawa, Poland

The Heusler alloys $Co_2Mn_{1-x}Fe_xSi$ have recently attracted particular interest due to the unique possibility to tune the spin polarization by varying the Mn/Fe fraction. The calculated band structures show the shift of the Fermi energy from the top of the minority valence band for Co_2MnSi to the bottom of the minority conduction band for Co_2FeSi upon Fe doping. From computational results it has been

predicted that a compound with an intermediate Fe concentration of about 50% should be best suited for spintronic applications. These theoretical findings still require experimental proofs. We report on ^{57}Fe Mössbauer spectroscopic, ^{59}Co and ^{55}Mn NMR studies of hyperfine magnetic fields (HFF) in $Co_2Mn_{1-x}Fe_xSi$ ($0 \leq x \leq 1$). The hyperfine magnetic field on Fe atoms is non-monotonic and shows maximum at $x = 0.5$. We argue that the maximum value of the HFF found on Fe and Co atoms at $x = 0.5$ is due to the existence of maximal spin-polarization in $Co_2Mn_{0.5}Fe_{0.5}Si$. Experimentally found HFF values are compared with results following from electronic band structure calculations taking into account electronic correlations (LDA+U).

MA 8.7 Mon 16:45 H22

A spatially resolved investigation of the local, micro-magnetic domain structure of single and polycrystalline Co_2FeSi. — •Andrei Gloskovskii[1], Joachim Barth[1], Benjamin Balke[1], Gerhard Fecher[1], Claudia Felser[1], Florian Kronast[2], Ruslan Ovsyannikov[2], and Gerd Schönhense[3] — [1]Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg - Universität Mainz, D-55099 Mainz, Germany — [2]BESSY GmbH, Albert-Einstein-Straße 15, 12489 Berlin, Germany — [3]Institut für Physik, Johannes Gutenberg - Universität Mainz, D-55099 Mainz, Germany

The Heusler compound Co_2FeSi is a promising material for magneto-electronic devices. With a Curie temperature of 1100 K and a saturation magnetisation of 6 Bohr magnetons and a high spin polarisation at the Fermi edge it fulfils the essential requirements for magnetic sensors or spin valve structures. An essential feature for such devices is the micro-magnetic domain structure. XMCD-PEEM has been used for a direct observation of the domain structure of single- and polycrystalline samples. The (110)-oriented surface of the single crystal exhibits a multi-domain pattern characteristic for systems with an easy axis that might point out of the surface. Spin polarised photo emission from a single domain of the single crystal shows a spin polarisation of 16% at the Fermi energy and up to 35% in the d-bands, at room temperature.

MA 8.8 Mon 17:00 H22

Sr_2CrOsO_6: Spin polarized metal-insulator transition by $5d$ band filling — Yoshiharu Krockenberger[1,2], Kaylash Mogare[2], Manfred Reehuis[2,3], Martin Tovar[3], Martin Jansen[2], Ganapathy Vaitheeswaran[4], Venkata Kanchana[4], Anna Delin[4], Fabrice Wilhelm[5], Andrei Rogalev[5], Andreas Winkler[1], and •Lambert Alff[1] — [1]Institut für Materialwissenschaft, TU Darmstadt — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart — [3]Hahn-Meitner-Institut, Berlin — [4]Department of Materials Science and Engineering, KTH Stockholm — [5]European Synchrotron Radiation Facility (ESRF), Grenoble

In the search for new spintronic materials with high spin-polarization at room-temperature, we have synthesized an osmium based double perovskite with a Curie-temperature of 725 K. Our combined experimental results confirm the existence of a sizable induced magnetic moment at the Os site, supported by band-structure calculations in agreement with a proposed kinetic energy driven mechanism of ferrimagnetism in these compounds. The intriguing property of Sr_2CrOsO_6 is that it is at the endpoint of a metal-insulator transition due to $5d$ band filling, and at the same time ferrimagnetism and high-spin polarization is preserved.

[1] Y. Krockenberger, K. Mogare, M. Reehuis, M. Tovar, M. Jansen, G. Vaitheeswaran, V. Kanchana, F. Bultmark, A. Delin, F. Wilhelm, A. Rogalev, A. Winkler, and L. Alff. Phys. Rev. B, Rapid Comm. (2007).