MA 25: Magnetic Heusler Compounds

Time: Wednesday 9:30–12:30 Location: H10

MA 25.1 Wed 9:30 H10

Crystal growth of $Co_2Cr_xFe_{1-x}Al$ Heusler compounds — •Ahmad Omar, Maria Dimitrakopoulou, Christian George Friedrich Blum, Horst Wendrock, Steven Rodan, Silke Hampel, Wolfgang L öser, Bernd B üchner, and Sabine Wurmehl — Leibniz Institute for Solid State and Materials Research, D-01171 Dresden, Germany

Heusler compounds find extensive application as materials for magnetic tunnel junctions and memory devices as many are predicted to be half-metallic ferromagnets and hence have much potential in spintronics. Unfortunately, data for thin films as well as bulk materials for many compositions are fraught with anomalies. The present work primarily highlights crystal growth of select Heusler compounds ($Co_2Cr_xFe_{1-x}Al$) as an attempt towards understanding the interplay between the structure and intrinsic properties. We have used the Optical Floating Zone technique for the growth process. Apart from a phase segregation in the as cast samples, a spinodal decomposition of the grown samples has been observed for compounds containing Cr. The extent and the effect of the spinodal decomposition has also been studied.

MA 25.2 Wed 9:45 H10

Electronic structure of Fe2CrSi beyond the generalized gradient approximation — •Markus Meinert — Thin Films and Physics of Nanostructures, Department of Physics, Bielefeld University, 33615 Bielefeld, Germany

The ferromagnetic Heusler compound Fe_2CrSi has been predicted to be a half-metal from standard density functional theory calculations [1,2]. In the present study, we investigate the properties of Fe_2CrSi beyond the level of the generalized gradient approximation (GGA) within density functional theory. We compare the LDA, several GGAs, meta-GGAs including the Tran-Blaha modified Becke-Johnson potential (mBJLDA), hybrid functionals, the $+U$ method, and one-shot GW. The TPSS and M06-L functionals, the mBJLDA model potential, GGA+U, and the hybrids predict Fe_2CrSi consistently as a semiconductor with a small majority and a larger minority gap. In most semilocal approximations we find a ferromagnetic groundstate, but M06-L, GGA+U, HSE06, and PBE0 predict Fe_2CrSi to be a ferrimagnet. The sensitivity of the groundstate of Fe_2CrSi makes this compound an ideal test case to assess the validity of the various available approximations for the density functional for the material class of $3d$ transition metal based Heusler compounds.

[1] Ishida et al., Mater. Trans. **47**, 464 (2006). [2] Luo et al., J. Phys. D: Appl. Phys. **40**, 7121 (2007).

MA 25.3 Wed 10:00 H10

Transport Investigations of Mn_3Si — •Frank Steckel, Steven Rodan, Regina Hermann, Christian G.F. Blum, Sabine Wurmehl, Bernd Büchner, and Christian Hess — Leibniz Institute for Solid State and Materials Research, Dresden, Deutschland

We investigate electronic and thermal transport phenomena of the itinerant antiferromagnet Mn_3Si, which has been suggested to be a prototype material for realizing half-metallic antiferromagnetism [1] with a spin density wave below 25 K. We measured a complete set of transport coefficients: the resistivity, the Hall effect as well as the thermal conductivity, the thermopower and the Nernst effect in the temperature range from 10 K up to 300 K. In the vicinity of the antiferromagnetic transition temperature we found pronounced anomalies in the transport coefficients and a large fluctuation regime which extends to temperatures much higher (up to about 150 K) than the antiferromagnetic ordering temperature.

[1] C. Pfleiderer et al., Phys. Rev. B 65 (2002) 172404

MA 25.4 Wed 10:15 H10

X-ray absorption spectroscopy and magnetic circular dichroism studies of $L1_0$-Mn-Ga thin films — •Manuel Glas[1], Daniel Ebke[2], Christian Sterwerf[1], Jan Schmalhorst[1], Catherine Jenkins[3], Elke Arenholz[3], and Günter Reiss[1] — [1]Thin Films and Physics of Nanostructures, Bielefeld University, Germany — [2]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany — [3]Advanced Light Source Berkeley, CA, USA

The continuous miniaturization process for spintronic devices requires consistently new materials. In particular, materials with high spin polarization, high Curie temperature, high perpendicular magnetic anisotropy, low magnetic moment, and low magnetic damping have found a lot of interest, due to the predicted lower current densities for spin torque transfer switching. The tetragonally distorted $Mn_{3-x}Ga$ compound fulfils these properties and is therefore a promising candidate for STT-switching MRAM devices. To achieve a high TMR effect the interface between the electrodes and barrier plays an important role. Therefore we investigated the interface between a $Mn_{64}Ga_{36}$ electrode and a 2.3 nm thick MgO barrier by element specific X-ray absorption spectroscopy (XAS) and magnetic circular dichroism (XMCD). Additionally, we examined the effects of CoFeB sandwiched between the Mn-Ga and the MgO with different thicknesses, and the deposition method for the MgO capping layer on the formation of interfacial MnO. Element specific full hysteresis loops were taken to determine the easy magnetization axis of the Mn and Co, respectively.

MA 25.5 Wed 10:30 H10

Basic investigations of hard magnetic binary $Mn_{(3-x)}Ga$ bulk materials — •Hannes Stummer, Christian Blum, Wolfgang Löser, Sabine Wurmehl, and Bernd Büchner — Leibniz Institut für Festkörper- und Werkstoffforschung Dresden, Germany

Polycrystalline materials from the manganese rich part of the Manganese-Gallium phase system provide hard magnetic properties with high coercive fields and low saturation.[1] These binary intermetallic Heusler-type compounds assume as starting material for new permanent magnetic materials.[2] The presented investigations deal with the polycrystalline compounds, their micro- and crystal structure analysis in addition to the magnetic properties. The fundamental studies give information about the phase formation in the complex binary phase system of Mn-Ga. Also a new promising synthesis route for the crystallization of single-crystalline samples, needed for comprehensive magnetic measurements, is presented. Furthermore it is shown that by slightly changing of the material composition new permanent magnetic materials can be produced. [1]Balke et al., Appl. Phys. Lett. 90, 152504 (2007) [2]Winterlik et al., Physical Review B, 77, 054406 (2008)

MA 25.6 Wed 10:45 H10

Electronic properties of Heusler alloys investigated by X-ray magnetic linear dichroism — •Mirko Emmel[1], Ingo Krug[2], Daniel Gottlob[2], Alexey Alfonsov[3], Sabine Wurmehl[3], Hans-Joachim Elmers[1], and Gerhard Jakob[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany — [2]Forschungszentrum Jülich, Germany — [3]Leibniz-Institut für Festkörper- und Werkstoffforschung IFW-Dresden, Dresden, Germany

Theoretical calculations have indicated that XMLD spectra are much more sensitive to changes of the electronic structure compared to XMCD spectra [1]. Thus several thin films of Co_2FeSi have been prepared on a MgO(100) substrate to verify existing theoretical predictions. The films were prepared by DC magnetron sputtering at varying deposition temperatures to achieve different degrees of atomic order within the films. After a capping layer of Al or Cr was deposited to prevent oxidation, the samples were analyzed by NMR measurements at IFW Dresden. The XMLD measurements were performed using the XAS apparatus installed at the UE56-1/SGM beamline (Jülich). The results show clear and uniform features. However, the samples capped with Al show similar behavior to results for $Co_2FeAl_{0.5}Si_{0.5}$. Thus it is presumed that Al atoms are being implanted into the subsurface of Co_2FeSi, which makes Cr the capping layer of choice. Finally we see a change of the magnitude within the XMLD spectra depending on the local atomic order of the film.

We acknowledge support by DFG research group ASPIMATT.

[1] M. Kallmayer et al., Phy. Rev. B 84, 054448 (2011)

MA 25.7 Wed 11:00 H10

Spin-wave instabilities in a micro-structured $Co_2Mn_{0.6}Fe_{0.4}Si$ Heusler waveguide — •Philipp Pirro[1], Thomas Sebastian[1,2], Thomas Brächer[1,2], Alexander A. Serga[1], Takahide Kubota[3], Hiroshi Naganuma[4], Mikihiko Oogane[4], Yasuo Ando[4], and Burkard Hillebrands[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Graduate School Materials Science in

Mainz, Gottlieb-Daimler-Straße 47, 67663 Kaiserslautern, Germany — [3]WPI Advanced Institute for Materials Research, Tohoku University, Katahira 2-1-1, Aoba-ku, Sendai 980-8577, Japan — [4]Department of Applied Physics, Graduate School of Engineering, Tohoku University, Aoba-yama 6-6-05, Sendai 980-8579, Japan

Magnetic Heusler compounds are expected to show novel nonlinear magnonic transport phenomena due to very low Gilbert damping and high decay length for spin-waves [1] for some of these materials.

We present a nonlinear instability of propagating spin waves in the Heusler compound $Co_2Mn_{0.6}Fe_{0.4}Si$ which couples the initial spin wave (frequency f_{MW}) with two modes of different frequencies f_1 and f_2. As the separation $\Delta f = f_{MW} - f_1$ can reach more than 4 GHz, automodulation effects can be excluded and we interpret our observations as a kinetic instability.

We acknowledge support by the OPTIMAS Carl-Zeiss doctoral program, the DFG Research Unit 1464 and the Strategic Japanese-German Joint Research from JST: ASPIMATT.

[1] T. Sebastian, et al., Appl. Phys. Lett. 100, 112402 (2012).

MA 25.8 Wed 11:15 H10

NMR Sheds Light on Structural Evolution upon Annealing and Off-Stoichiometry in Nominal Co_2MnSi Thin Films — •Steven Rodan[1], Alexey Alfonsov[1], Maria-Eleni Belesi[1], Filippo Ferraro[2], Jürgen T. Kohlhepp[2], Henk J. M. Swagten[2], Bert Koopmans[2], Bernd Büchner[1], and Sabine Wurmehl[1] — [1]Leibniz Institute for Solid State and Materials Research, 01171 Dresden, Germany — [2]Eindhoven University of Technology, 5600 MB Eindhoven, Netherlands

Half-metallic ferromagnets (HMFs), with fully spin-polarized conduction electrons, are prime candidates for developing spintronic devices. Many Heusler compounds, such as Co_2MnSi, are predicted to be HMFs. A local probe technique such as nuclear magnetic resonance (NMR) is essential for understanding the microscopic origin of manifested physical properties, such as the magnetoresistance ratio measured in giant magnetoresistance (GMR) devices. Using NMR we have studied the evolution of local atomic structure in numerous Co_2MnSi thin films prepared by different methods, subjected to various annealing temperatures, and with varying stoichiometry. For all cases, we investigated models for different types of disorder, and quantitatively deduced the off-stoichiometry. By understanding how the local structure affects the physical properties, one can hope to control and optimize the properties which are of interest for spintronics by appropriately tuning the structure.

MA 25.9 Wed 11:30 H10

Cubic phase in Fe_2-based Heusler materials stabilized by disorder. — •Janos Kiss[1], Stanislav Chadov[1], Gerhard H. Fecher[1], Teuta Gasi[2], Vadim Ksenofontov[2], Peter Adler[1], and Claudia Felser[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden — [2]Johannes-Gutenberg Universität, Mainz

Due to their relatively large magnetic moments and strong magnetic anisotropy, the Fe_2-based Heusler compounds with tetragonal distortion are expected to be attractive candidates in hard-magnetic applications. In contrast to the first theoretical predictions, however, many of them crystallize in the cubic structure. In the framework of *ab-initio* electron structure calculations, we explain the stability of their cubic phase as based on combined effect of intrinsic chemical disorder and crystal symmetry.

MA 25.10 Wed 11:45 H10

Giant non-collinear magnetism and a spin reorientation in Mn_2RhSn Heusler compound. — •Olga Meshcheriakova[1,2], Ajaya K. Nayak[3], Stanislav Chadov[3], Jürgen Kübler[4], Teuta Gasi[1], Vadim Ksenofontov[1], Walter Schnelle[3], Alexander Tsirlin[3], and Claudia Felser[1,2,3] — [1]Institut für Anorganische und Analytische Chemie, Johannes Gutenberg Universität Mainz, 55099 Mainz, Germany — [2]Graduate School of Excellence Materials Science in Mainz, 55128 Mainz, Germany — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany — [4]Institut für Festkörperphysik, Technische Universität Darmstadt, 64289 Darmstadt, Germany

Magnetic, structural, heat and transport properties of the bulk polycrystalline Mn_2RhSn tetragonal Heusler compound have been investigated. A field-driven magnetic transition was observed within a temperature range between 50 and 100 K. Such behavior was attributed to the non-collinear magnetism which results as competition between the anisotropy induced by tetragonal strain and typical antiparallel alignment of two Mn magnetic sublattices. According to the additional first-principles calculations, the present material exhibits a huge angle between these two magnetic sublattices. The experimentally measured saturated magnetization (of 2 μ_B per formula unit) was reasonably explained by combining the non-collinear magnetic calculations with the effects of an antisite disorder indicated by Moessbauer measurements.

This work is supported by the Graduate School of Excellence Materials Science in Mainz (MAINZ).

MA 25.11 Wed 12:00 H10

Different stacking of square layers in tetragonal Heusler compounds (Mn_3X, X=Ga, Ge, Sn) with perpendicular magnetization — •S.-C. Wu, G. H. Fecher, and C. Felser — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Tetragonal Mn_3X (X=Ga, Ge, Sn) compounds attracted attention because of the perpendicular magnetization in thin films. The tetragonal Heusler structure can be built by stacking of square layers. The type of stacking maybe controlled by the conditions at the thin film growth. The most interesting property of binary Heusler alloys Mn_3X with tetragonal structure is the magneto-crystalline anisotropy (MCA). Consider layers as follows: A contains Mn and X, in A' the positions of Mn and X are exchanged, and B contains only Mn. The tetragonal Heusler type binaries (Al_3Ti-type) are build by ABA'B stacking of square layers, whilst ABAB stacking results in the $CuTi_3$-type structure. Calculations were performed for both type of structures. The perpendicular magneto-crystalline anisotropy in the $CuTi_3$ structure was found to be E_{MCA} = 0.82, 0.95, 1.22 meV for Mn_3Ga, Mn_3Ge, Mn_3Sn. Those values make them promising MCA materials. Furthermore, we report crystalline, electronic, and magnetic structure as well as elastic properties of the compounds.

MA 25.12 Wed 12:15 H10

Magnetic properties of Heusler nanocrystals inside carbon nanotubes — •Markus Gellesch, Maria Dimitrakopoulou, Maik Scholz, Sabine Wurmehl, Silke Hampel, and Bernd Büchner — Leibniz Institut für Festkörper- und Werkstoffforschung Dresden

Magnetic properties of nanoscale systems may differ largely from the magnetism in the respective bulk phase and thus can lead to the emergence of interesting and also novel physical properties. Here we present results of investigations of thermomagnetic properties of Heusler nanoparticles prepared inside multi-walled carbon nanotubes via a wet-chemical approach. We observe chemical stable Co_2FeGa nanoparticles with a narrow diameter distribution, a high degree of crystallinity and with a well-defined stoichiometry within the experimental error. Our study shows, that the coercive field of the Heusler nanocrystals inside carbon nanotubes is greatly enhanced and depends on the mean diameter of the Heusler nanocrystals, while the saturation magnetic moment known from the bulk phase is preserved. The results of our work open the door for the exploration of Heusler materials at the nanoscale and also guide the way to the synthesis of nano materials with tailored physical properties.