MA 15: Magnetic Heuslers, Half-metals and Oxides (jointly with TT)

Time: Monday 15:00–18:30 Location: HSZ 403

MA 15.1 Mon 15:00 HSZ 403

Giant anomalous Hall effect in Heusler compounds — •Kaustuv Manna[1], Rolf Stinshoff[1], Ting-Hui Kao[1], Nitesh Kumar[1], Chandra Shekhar[1], Jayita Nayak[1], Sunil Wilfred DSouza[1], Sanjay Singh[1], Gerhard H. Fecher[1], Stuart S. P. Parkin[2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany

The Co-Based Heusler compounds have drawn considerable interest in last few years for the spintronics application due to the prediction of large anomalous Hall effect (AHE) as well as spin Hall effect [1]. For many of the samples like Co_2MnAl, Co_2MnGa etc. formation of the Weyl points near Fermi energy was proposed to be the origin for such fascinating behaviour [2]. Here we report the giant anomalous Hall effect in Co_2MnGa single crystals. The sample crystallizes with $Fm\bar{3}m$ which hold the inversion symmetry and the AHE observed $\sim$ 1200 S cm^{-1} at 2 K. The ferromagnetic moment found $\sim$ 4.23 μ_B/fu. On the contrary, for the systems where the inversion symmetry is broken, like Mn_2CoGa [$F\bar{4}3m$], there is no Weyl point in the band structure. Interestingly we don't observe any AHE at 2 K though the system possess ferromagnetic moment of $\sim$ 2.27 μ_B/fu.

[1]Jen-Chuan Tung and Guang-Yu Guo, New J. Phys. **15**, 033014 (2013).
[2]J. Kubler and C. Felser, Europhys. Lett. **114**, 47005 (2016).

MA 15.2 Mon 15:15 HSZ 403

Magnetic field assisted heat treatment — •Franziska Seifert[1], Bernd Büchner[1,2], and Sabine Wurmehl[1] — [1]Leibniz Institute for Solid State Research Dresden, Germany — [2]Technische Universität Dresden, Germany

The convetionell way to improve or tailor the structural and physical properties of a material is, in most of the cases, high temperature annealing. It is also possible to anneal the material at a certain magnetic field at room temperature. With our device we combine both, magnetic field and high temperature treatments. We are able to tailor the magnetic properties by applying a magnetic field during high temperature annealing. Especially in multiphase materials, we can favour particular one phase, which determines the magnetic properties. This annealing technique is very interesting for shape memory alloys, magnetocaloric, hardmagnetic or highly spin polarized materials. Our preliminary results will be discussed.

MA 15.3 Mon 15:30 HSZ 403

Stability of a highly spin polarized surface resonance of Co_2MnSi at spin-valve interfaces — •Christian Lidig[1], Alexander Kronenberg[1], Andrei Gloskovskii[2], Mathias Kläui[1], and Martin Jourdan[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany — [2]Deutsches Elektronen-Synchrotron DESY, 22603 Hamburg, Germany

The magnitude of the spin polarization of ferromagnetic materials is a key property for their application in spin transport-based electronics. However it is not the bulk, but the interface of the material, which is relevant for applications. Investigating thin films of Co_2MnSi (CMS) by spin-resolved UPS and spin-integrated HAXPES, we recently observed a high spin polarization at room temperature in a wide energy range below the Fermi energy, which is related to a stable highly spin polarized surface resonance[1,2]. Correspondingly, CMS / Ag / CMS spin valves show large GMR values[3]. However, the use of alternative spacer layers like Cr[4] always resulted in strongly reduced GMR values. A characteristic spectral feature close to the Fermi edge in HAXPES is related to the surface resonance[1]. This spectral feature is completely suppressed at CMS interfaces with Al and Cr and diminished in combination with Cu. However, it is fully conserved at epitaxial interfaces with Ag, explaining the superior magnetoresistance of spin-valves with this materials combination. [1] M. Jourdan et al., Nat. Commun. **5**, 3974 (2014). [2] J. Braun et al., Phys. Rev. B **91**, 195128 (2015). [3] Y. Sakuraba et al., Appl. Phys. Lett. **101**, 252408 (2012). [4] K. Yakushiji et al. Appl. Phys. Lett. **88**, 222504 (2006).

MA 15.4 Mon 15:45 HSZ 403

Defect-induced magnetic structure of CuMnSb — •Frantisek Maca[1], Josef Kudrnovsky[1], Vaclav Drchal[1], and Ilja Turek[2] — [1]Institute of Physics ASCR, Praha, Czech Republic — [2]Charles University, Faculty of Mathematics and Physics, Praha, Czech Republic

We have investigated the magnetic phases of CuMnSb Heusler alloy with defects which exist in real experimental conditions. Total energy calculations confirm that the AFM[100]-phase is the ground state for the ideal CuMnSb in contrast to the experimentally observed AFM[111]-phase. Calculated formation energies indicate as possible candidates for defects the Cu-Mn swaps for the stoichiometric alloy and Mn-antisites on Cu-lattice and Mn-interstitials for Mn enriched alloys.

The total energies of various magnetic phases of CuMnSb with defects were determined using two different structural models, namely, the full-potential supercell approach and the alloy model employing the coherent potential approximation (CPA). We have found that the AFM[111]-ground state is stabilized for a low critical impurity concentrations approximately 3% . We have also investigated the influence of defects on the exchange interactions among Mn-moments and the stability of magnetic order by using the Heisenberg model Hamiltonian. The stability of the AFM[111] phase is in all cases enhanced by electron correlations in narrow Mn-bands treated here in the static limit (LDA+U).

MA 15.5 Mon 16:00 HSZ 403

Magnetotransport in Half-Metallic Manganese Ruthenium Gallium — •Ciaran Fowley[1], Kiril Borisov[2], Gwenael Atcheson[2], Yong-Chang Lau[2], Naganivetha Thiyagarajah[2], Rodolfo Gallardo[3], Jurgen Lindner[1], Zhaosheng Wang[4], Erik Kampert[4], Mike Coey[2], Plamen Stamenov[2], Karsten Rode[2], and Alina Maria Deac[1] — [1]Institute for Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328, Germany — [2]AMBER and School of Physics, Trinity College Dublin, Dublin 2, Ireland — [3]Universidad Técnica Federico Santa María, Valparaíso, Chile — [4]High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, 01328, Germany

The recently discovered fully-compensated half-metal, manganese-ruthenium-gallium (MRG), is a very promising material for spintronics. It possesses tunable magnetic moment, high magnetic anisotropy field and high spin polarisation. Here, we use the extraordinary Hall effect and longitudinal magnetoresistance to characterise the properties of MRG. Experiments are carried out in pulsed magnetic fields up to 60 T at the Dresden High Magnetic Field Laboratory (HLD). The spin-flop transition, as well as a large spontaneous Hall angle (over 2%) is observed. The magneto-transport in MRG is shown to be dominated by one sublattice only. The spontaneous Hall angle is non-zero even at the magnetic compensation temperature (i.e. when the total magnetic moment is zero). MRG behaves magnetically like an antiferromagnet and electrically as a normal ferromagnet with a sizeable spin-polarisation.

MA 15.6 Mon 16:15 HSZ 403

Tunneling Magnetoresistance in MnRuGa based Magnetic Tunnel Junctions — •Aleksandra Titova[1,2], Ciaran Fowley[1], Kiril Borisov[3], Davide Betto[3], Yong Chang Lau[3], Nivetha Thiyagarajah[3], Gwenael Atcheson[3], Michael Coey[3], Plamen Stamenov[3], Karsten Rode[3], Jürgen Lindner[1], Jürgen Fassbender[1,2], and Alina Deac[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Technische Universität Dresden, Germany — [3]Trinity College, Dublin, Dublin, Ireland

Some intermetallic Heusler compounds display high spin polarization and low magnetic moment. Thin-film samples can possess huge uniaxial anisotropy fields, exceeding tens of teslas. This, combined with their tuneable properites, make these materials very attractive for THz based spin-transfer-torque oscillators. Recently new material from this family was discovered - MnRuGa (MRG) - the first experimentally achieved fully-compensated half-metallic ferrimagnet. Here we show that MRG can be integrated in perpendicular anisotropy magnetic tunnel junctions stacks. Tunneling magnetoresistance (TMR) ratios up to 40% are observed. We also demonstrate that the TMR exists even when the net magnetization of MRG is strictly zero, implying that, at compensation, MRG exhibits a sizable spin polarization. The

role of different diffusion barrier layers between MRG and the tunneling barrier as well as annealing temperature was investigated.

This work is supported by the Helmholtz Young Investigator Initiative Grant No. VH-N6-1048.

15 min. break.

MA 15.7 Mon 16:45 HSZ 403

Influence of grain boundaries on cohesive and magnetic properties in the inverse Heusler phase Fe_2CoGa

— •Georg Krugel, Daniel Urban, Wolfgang Körner, and Christian Elsässer — Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

Heusler phases are promising candidates in the search for a rare-earth free hard-magnetic compound allowing high Curie temperatures. Experimentally, they are often found to be brittle and the effect of their microstructure on the material properties is not yet understood in detail.

Using DFT calculations we investigate the effect of grain boundaries (GB) on the mechanical and magnetic properties of the inverse Heusler phase Fe_2CoGa as a case study. Four different GBs are studied and several different translation states taken into account for each of them to sample the gamma surface. The GB excess volume, the formation energy of the GB and the cohesion energies of the grains are calculated and compared in order to shed more light onto the influence of GB on the mechanical properties of Heusler phases. For an understanding of the behaviour of magnetism at the GB the local atomic configurations are analysed together with the atomic magnetic moments. Moreover, we calculate the magnetic anisotropy energies for the energetically most favorable configurations. Our results support experimental efforts to determine tailored synthesis routes.

MA 15.8 Mon 17:00 HSZ 403

Study of compensated ferrimagnetic Heusler materials $Mn_{3-x}Pt_xGa$

— •Vivek Kumar[1], Ajaya K. Nayak[1,2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany

Compensated ferrimagnets with large spin polarization and high ordering temperature are perfect candidates for realization of antiferromagnetic spintronics. These materials with additional perpendicular magnetocrystalline anisotropy can be ideal candidates for spin transfer torque applications. In this direction Heusler materials find special attention where chemical disorder can be used as an engineering tool to improve desired properties. The tetragonal Mn_3Ga is an interesting candidate as a starting material which exhibits a high Curie temperature (T_C). It is theoretically predicted that substitution of Mn with a late transition metal can lead to a decrease in the total magnetic moment [1]. Here we present the structural and magnetic properties of single phase bulk tetragonal $Mn_{3-x}Pt_xGa$ Heusler materials for x varying from 0 to 0.6. We have found that the tetragonal distortion increases with increasing Pt concentration, indicating stabilization of the tetragonal phase with Pt substitution. With increasing Pt concentration the total magnetic moment systematically decreases and reach a compensation point around x=0.6. Although the magnetic ordering temperature displays a slight reduction with Pt substitution the compensated sample exhibits a T_C well above room temperature.

[1]R. Sahoo *et al.*, Adv. Mat. **28**, 8499 (2016).

MA 15.9 Mon 17:15 HSZ 403

High quality Yttrium Iron Garnet thin films by room temperature deposition and annealing in argon atmosphere

— •Christoph Hauser[1], Christian Eisenschmidt[1], Hakan Deniz[2], and Georg Schmidt[1,3] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [3]Interdisziplinäres Zentrum für Materialwissenschaften, Halle, Germany

We have recently [1] shown that depositing Yttrium Iron Garnet by Pulsed Laser Deposition at room temperature and subsequent annealing in an oxygen atmosphere results in fully epitaxial layers. The layers show extremely low damping and very narrow linewidth in Ferromagnetic Resonance, even for thin layers. Here we show that annealing in oxygen is not mandatory. Also annealing in argon results in high quality layers. For a 63 nm YIG layer a linewidth of 2.26 Oe @ 9.6GHz and a damping of $1.61 \cdot 10^{-4}$ is observed in FMR. Structural characterization indicates high crystalline quality and no visible defects. [1] Hauser *et al.*, Sci. Rep. 6, 20827 (2016)

MA 15.10 Mon 17:30 HSZ 403

Colossal increase in the magnetic moment of NiCo2O4 films via He-ion irradiation

— •Parul Pandey[1], Yugandhar Bitla[2], Matthias Zschornak[1], Mao Wang[1], Chi Xu[1], Joerg Grenzer[1], Sibylle Gemming[1], Manfred Helm[1], Ying-Hao Chu[2,3], and Shengqiang Zhou[1] — [1]Helmholtz-Zentrum-Dresden -Rossendorf, Dresden, Germany — [2]National Chiao Tung University, Hsinchu, Taiwan — [3]Institute of Physics, Academia Sinica, Taipei, Taiwan

The spinel NiCo2O4 exhibits the unique combination of electrical conductivity, infrared transparency, electro catalytic activity, and ferrimagnetic order, which makes it an attractive material for spintronic applications. The NiCo2O4 thin-films electrical and magnetic properties can be manipulated from high temperature ferrimagnetic and metallic to low temperature ferromagnetic and insulating by changing the growth temperature. The high-quality epitaxial NiCo2O4 films were grown on MgAl2O4 (100) substrate at ~ 400°C exhibits metallic behavior accompanied by ferrimagnetic order with moment ~ 2 μB/fu. Here, we report the impact of He-ion irradiation with fluence ranging from 5*1015/cm2 - 3*1016/cm2 on these metallic NiCo2O4 films. The use of He-ion irradiation results in the coherent control of out-of-plane lattice parameter of these films without changing its in-plane lattice parameter. The comprehensive study of magnetization data reveals the magnetic moment in the irradiated films increases drastically to ~ 4 μB/fu. The X-ray absorption spectroscopic study also suggests the possible charge redistribution within the octahedral sites of the NiCo2O4 films which corroborate well with the increase in the magnetic moment.

MA 15.11 Mon 17:45 HSZ 403

Magnetic and structural properties in the spin-dimer system Ba0.1Sr2.9Cr2O8

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Sr3Cr2O8 and Ba3Cr2O8 are two insulating dimerizad antiferromagnets with the magnetic ions, Cr 5+, that lie on hexagonal bilayers with strong intradimer antiferromagnetic interaction. This leads to a singlet ground state and gapped triplet states. Intradimer interaction constant J0 strongly depends on the stoichiometry.

We report on the change of the structural and magnetic properties of a spin-dimer system, Sr3Cr2O8, by introducing chemical disorder. Two large single crystal of Ba(3-x)Sr(x)Cr2O8 with x=2.9 and x=2.8 have been grown in a four-mirror type optical floating-zone furnace. By performing magnetization, heat-capacity measurements we have studied structural and magnetic properties of these compounds. Our inelastic neutron scattering measurements of spin-dimer compound Ba0.1Sr2.9Cr2O8 determine the interaction constants and the spin gap. The intradimer interaction constant is found to be J0=5.327(1) meV, that about 8% smaller than for pure Sr3Cr2O8 compound. Spin gap is decreasing about 6% with introducing chemical disorder.

MA 15.12 Mon 18:00 HSZ 403

First principles study of orbital order in Mn doped FeV2O4

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The long range orbital order in vanadium spinel oxides has been thoroughly debated by condensed matter physicists in recent years. MnV_2O_4 and FeV_2O_4 are two such compounds where the debate is centered around whether there are complex or real orbitals involved in the ordering process. In this context, we have investigated the long range orbital order in Mn doped FeV_2O_4 as a function of Mn doping (x). We have employed first-principles density functional theory (DFT) including Coulomb correlation (GGA+U) and spin-orbit interaction (GGA+U+SO) as well as the wannierization of our DFT derived vanadium d-bands for our analysis of the orbital order in these systems. We observe that for x≤0.6, the orbital order at V sites consists of a linear superposition of d_{xz} and d_{yz} orbitals of the type dxz±dyz whereas for x > 0.6, A-type ordering is observed. The effect of spin-orbit interaction on orbital ordering is found to be not significant in the entire range of doping studied indicating the absence of complex orbitals in the ordering[1]. We also analyze the orbital ordering from the Raman spectrum calculated using ab-initio phonon within the DFT framework and compare the same with the experimental observations.

Reference: [1] Dibyendu Dey, T. Maitra, and A. Taraphder; Phys. Rev. B 93, 195133 (2016)

MA 15.13 Mon 18:15 HSZ 403

Curie temperature of ultra-thin EuO films in proximity to a metal — Brian Tam, Andreas Reisner, Steffen Wirth, •Simone G. Altendorf, and Liu Hao Tjeng — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

A reduction of the thickness of ferromagnetic layers towards the ultra-thin limit goes along with a strong reduction of the Curie temperature thereby hindering potential technological applications. We study the possibility to compensate the lowering of the magnetic ordering temperature of ultra-thin EuO films by bringing them in close proximity to a metal, thereby trying to make use of the so-called image charge screening effect to increase the strength of the magnetic exchange interactions. We utilize the well-established Eu-distillation-assisted MBE growth method to prepare highly stoichiometric EuO films on YSZ substrates. By capping one half of each film with a Mg metal overlayer and the other half with MgO, we were able to directly determine the effectiveness of the proximity effect of the metal to influence the magnetic properties of ultra-thin ferromagnetic films.