MA 5: Heusler compounds, semimetals and oxides (joint session MA/TT)

Time: Monday 9:30–13:15 Location: EB 301

MA 5.1 Mon 9:30 EB 301

Epitaxial growth of compensated ferrimagnetic Heusler thin films Mn-Fe-V-Al — •Siham Ouardi, Kazuya Z. Suzuki, and Shigemi Mizukami — WPI Advanced Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

Cubic Heusler compound $Mn_{1.5}FeV_{0.5}Al$ is a fully compensated half-metallic ferrimagnet with 24 valence electrons per formula unit. Here we report on epitaxial growth of the compensated ferrimagnetic Mn-Fe-V-Al Heusler films. The thin films of 30 nm thickness were grown directly on single crystalline MgO (001) substrates by using an ultra-high-vacuum magnetron sputtering technique. The Heusler structure was characterized by x-ray diffraction. The crystal structure ordering was controlled by the deposition at various substrate temperatures. Magnetometry measurements show a nearly vanishing magnetization where the anomalous Hall measurements exhibited magnetic ordering. The ferrimagnetic coupling between the different sublattices (Mn, Fe, and V) will discussed based on magnetic dichroism in angle-resolved hard X-ray photoelectron spectroscopy (MCD-HAXPES). The advantage of vanishing magnetization in combination with high spin polarization of this material thin films provides the possibility for spintronic device applications.

This work is supported by the Grant-in-Aid for Scientific Research KAKENHI (17H06513).

MA 5.2 Mon 9:45 EB 301

Polycrystalline vs Epitaxial Fe2-xMn1+xAl Heusler films with exchange bias shift — •Samer Kurdi[1], Giorgio Divitini[1], Massimo Ghidini[1,2,3], Markus Meinert[4], Marco Coïsson[5], Thomas Forrest[3], Günter Reiss[4], Sarnjeet Dhesi[3], Paola Tiberto[5], and Zoe Barber[1] — [1]University of Cambridge, UK — [2]Department of Physics, University of Parma, Italy — [3]Diamond Light Source, Oxfordshire, UK — [4]Center for Spinelectronic Materials and Devices, Bielefeld University, Germany — [5]INRIM, Torino, Italy

Magnetic recording devices are pervasive in current technology, and the development of environmentally friendly, sustainable and scalable devices based on Earth-abundant materials is a high research priority. In this study we investigate a simple, cost-effective single-layer exchange biased film for spin valves, a fundamental part of data storage systems.

We grew 200 nm polycrystalline and epitaxial Fe2-xMn1+xAl (x = -0.25, 0, 0.25) Heusler alloy films and characterized them to study the influence of Mn content on the exchange bias shift. The microstructure is shown to have a profound effect on film properties. In-situ annealing TEM studies show that the polycrystalline samples have Mn-rich and Fe-rich phases inducing a spin glass exchange bias shift of around 150 Oe at 4 K for Fe1.75Mn1.25Al. The exchange bias shift was observed at temperatures up to 12 K for the Fe1.75Mn1.25Al and up to 6 K for Fe2MnAl polycrystalline samples, whilst only the Fe1.75Mn1.25Al epitaxial film showed any bias shift (50 Oe, below 2 K). XMCD sum rule analysis of the polycrystalline samples showed different behaviour from the as-predicted perfectly ordered L21 Heusler structure.

MA 5.3 Mon 10:00 EB 301

Evolution of the interfacial perpendicular magnetic anisotropy constant of the Co_2FeAl interface upon annealing — •Andres Conca[1], Alessia Niesen[2], Guenter Reiss[2], and Burkard Hillebrands[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Center for Spintronic Materials and Devices, Physics Department, Bielefeld University, 33615 Bielefeld, Germany

We investigate a series of films with different thicknesses of the Heusler alloy Co_2FeAl in order to study the effect of annealing on the interface with a MgO layer and on the bulk magnetic properties. Our results reveal that while the perpendicular interface anisotropy constant $K_S^{\perp}$ is zero for the as-deposited samples, its value increases with annealing up to a value of 1.14 ± 0.07 mJ/m^2 for the series annealed at 320°C and of 2.0 ± 0.7 mJ/m^2 for the 450°C annealed series owing to a strong modification of the interface during the thermal treatment. This large value ensures a stabilization of a perpendicular magnetization orientation for a thickness below 1.7 nm. The data additionally shows that the in-plane biaxial anisotropy constant has a different evolution with thickness in as-deposited and annealed systems. The Gilbert damping parameter α shows an absolute minimum value of $2.8 \pm 0.1 \times 10^{-3}$. The thickness dependence is explained in terms of an inhomogeneous magnetization state generated by the interplay between the different anisotropies of the system and by the crystalline disorder.

Support by M-era.Net and HEUMEM is acknowledged.

MA 5.4 Mon 10:15 EB 301

high throughput screening for 3D spin gapless semiconductors in Heusler compounds — •qiang gao, ingo ophale, and hongbin zhang — Institute of Materials Science, TU Darmstadt, Darmstadt, Germany

In recent years, spin-gapless semiconductors (SGSs) have drawn intensive attention to the spintronics community. SGSs are half metals with the valence band maximum and conduction band minimum touching each other directly or indirectly (1). In this work, we performed high throughput screening for novel three-dimensional SGSs in quaternary Heusler compounds. Following the empirical rule, we focused on compounds with 18, 21 or 26 valence electrons (2). We have found many new Heusler compounds as candidate SGSs, with both direct and indirect touching. In particular, it is observed that spin-orbit coupling can also drive some systems into the SGS phase, resulting in possible interesting applications for future spintronic devices. (1) X.L. Wang, Phys. Rev. Lett., **100**, 156404 (2008). (2) X.T. Wang, Z.X. Cheng, J.L. Wang, X.L. Wang, G.D. Liu, J. Mater. Chem. C, **4**, 7176-7192 (2016).

MA 5.5 Mon 10:30 EB 301

Symmetry and magnitude of intrinsic spin-orbit torques in the half-Heusler alloy PtMnSb — •Johannes Mendil[1], Jan Krieft[2], Phuong Dao[1], Can Onur Avci[1], Myriam Haydee Aguirre[3], Karsten Rott[2], Jan-Michael Schmalhorst[2], Frank Freimuth[4], Günter Reiss[2], Timo Kuschel[2], and Pietro Gambardella[1] — [1]Department of Materials, ETH Zürich — [2]CSMD, Department of Physics, Bielefeld University — [3]Universidad de Zaragoza — [4]Peter Grünberg Institut, FZ Jülich

Magnetization manipulation by spin-orbit torques (SOTs) has advanced to an active research field over the past few years and is mostly focused on conventional ferromagnets deposited on heavy metal layers where the space inversion symmetry is broken at the interface[1]. However, space inversion symmetry is intrinsically broken in non-centrosymmetric crystals [2]. We present the first observation of intrinsic SOTs in PtMnSb single layers, which is a magnetic half-Heusler alloy. It was prepared by co-sputtering [3]. Using crystallographic symmetry, we separate the observed SOTs in odd and even components with respect to magnetization inversion. We reveal corresponding effective fields that scale up to the 2nd and 3rd power of magnetization components with a distinct symmetry compared to standard field-like and damping-like SOTs. Finally, we characterize the SOTs as a function of PtMnSb thickness and discuss the possibility of using PtMnSb for magnetic switching applications. [1] Garello et al., Nat. Nanotech. 8, 587 (2013) [2] Ciccarelli et al., Nat. Phys. 12, 855 (2016) [3] Krieft, Mendil et al., Phys. Stat. Sol. (RRL) 11, 1600439 (2017)

MA 5.6 Mon 10:45 EB 301

Electrical transport in the tetragonal Heusler system Mn-Pt-Ga — •Vivek Kumar[1], Ajaya K. Nayak[2], Nitesh Kumar[1], Peter Adler[1], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National Institute of Science Education and Research Bhubaneswar, Jatni, India

Nontrivial magnetic textures have attracted interest for improving desired properties in spintronic devices. Materials with non-centrosymmetric crystal structure are capable of inducing nontrivial spin structures due to the presence of Dzyaloshinskii-Moriya interaction (DMI). We have recently reported the magnetic antiskyrmions in tetragonal Heusler material $Mn_{1.4}Pt_{0.9}Pd_{0.1}Sn$ [1]. Here, we present the effect of spin-orbit interaction in another inverse tetragonal Heusler system Mn-Pt-Ga by electrical transport measurements. The tetragonal Mn_3Ga has ferrimagnetic order where Mn atoms sit on two different magnetic sublattices. The substitution of a late transition metal in place of Mn, here Pt, leads to breaking the inversion symmetry [2]. We found an anomaly in Hall resistivity which is dominating at higher Pt substitution. The behavior of Hall resistivity cannot be scaled with

magnetization. This is an indication of non-coplaner spin configurations in this system which are stabilized due to increase in DMI.
[1]A. K. Nayak *et al.*, Nature **548**, 561 (2017).
[2]S. Chadov *et al.*, Phys. Rev. B **91**, 094203 (2015).

MA 5.7 Mon 11:00 EB 301

Physical properties of the CuMnAs alloy - promising material for the antiferromagnetic spintronics — •Frantisek Maca[1], Josef Kudrnovsky[1], Vaclav Drchal[1], Karel Carva[2], Pavel Balaz[2], and Ilja Turek[2] — [1]Institute of Physics ASCR, Praha — [2]Faculty of Mathematics and Physics, Charles University, Praha

We have investigated from first principles the role of defects in the antiferromagnetic CuMnAs alloy with tetragonal structure [1]. Mn_{Cu}, Cu_{Mn}, Mn-Cu swaps, and vacancies on Mn- and Cu-sublattices are the most probable defects in this material. We have found that the electron correlations play important role in description of the phase stability.

We calculated transport properties for CuMnAs with defects of low formation energies and estimated in-plane resistivity of CuMnAs. Our numerical simulations fitted experiment very well if we assumed concentrations 3.5-5% Mn_{Cu} or Mn-Cu swaps, much larger concentrations would be needed for Cu_{Mn} defects or Mn-vacancies. We have estimated also the Neel temperature using the Monte Carlo approach, result agrees reasonably well with the experimentally observed value.

[1] F. Máca, J. Kudrnovský, V. Drchal, K. Carva, P. Baláž, and I. Turek, Phys. Rev. B **96** (2017) 094406.

15 minutes break

MA 5.8 Mon 11:30 EB 301

Improved reversibility by hydrostatic pressure in Ni-Mn based Heusler alloys — •Parul Devi[1], Luana Caron[1], Sanjay Singh[1], Alexandre Magnuu G. Carvalho[2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Laboratório Nacional de Luz Síncrotron, SáoPaulo, Brasil

Ni-Mn based Heusler alloys show first order diffusionless magnetostructural phase transition. The first order magnetostructural phase transition results in large magnetocaloric effect due to the change in both magnetic and crystal structure. The thermal or magnetic hysteresis is characteristic of first order phase transition which results in irreversibility of MCE. This irreversibility makes these materials less efficient for magnetic refrigeration. Therefore, nowadays, a lot of efforts have been made to reduce the hysteresis in these alloys [1]. In the present work, we observed a large reduction of hysteresis in off stoichiometric composition of Ni-Mn-In by hydrostatic pressure. To confirm that it is applicable to all Heusler alloys, we did it for two more different compositions of Ni-Mn based Heusler alloys. We got the decrement of hysteresis in these materials as well. However the rate of decrease in all three materials were different. Furthermore, we confirmed that the decrease in hysteresis was because of the increasingly geometric compatibility condition, recently predicted by James and co-workers [2].
[1]J. Liu *et al.*, Nature materials **11**, 620 (2012).
[2]Y. Song *et al.*, Nature Letter **502**, 85 (2013).

MA 5.9 Mon 11:45 EB 301

NMR investigations of irradiation-induced structural changes in Co_2MnSi thin films — •Franziska Hammerath[1], Mira R. D. Brandt[1], Rantej Bali[2], Kay Potzger[2], Roman Böttger[2], Rene Hübner[2], Yuya Sakuraba[3], Bernd Büchner[1], and Sabine Wurmehl[1] — [1]IFW Dresden, Institute for Solid State Research, Helmholtzstraße 20, 01069 Dresden — [2]Institute of Ion Beam Physics and Materials Research, HZDR, Bautzner Straße 400, 01328 Dresden, Germany — [3]National Institute for Materials Science (NIMS), Sengen 1-2-1, Tsukuba, Ibaraki 305-0047, Japan

Co_2MnSi is a well-known Heusler compound which is predicted to be half-metallic, i.e., possessing 100% spin-polarization and, thus, being a promising candidate material for enhancing the magneto-resistance of spin-valves [1]. Half-metallicity depends sensitively on the local chemical order, hence methods to improve the structure of Co_2MnSi towards the ideal $L2_1$ order and, thus, to achieve full spin-polarization are of huge technological relevance. On the basis of XRD measurements it has been argued that irradiation with He^+ ions induces an improvement of B2-order in Co_2MnSi thin films towards a possible formation of $L2_1$ order [2]. We investigated the structure-property relationship of He^+-irradiated Co_2MnSi alloy thin films locally by means of ^{59}Co nuclear magnetic resonance (NMR) and observed an increased disorder upon increasing the ion flux, going along with a decrease of the saturation magnetization.
[1] T. Iwase *et al.*, Appl. Phys. Express **2**, 063003 (2009).
[2] O. Gaier *et al.*, Appl. Phys. Lett. **94**, 152508 (2009).

MA 5.10 Mon 12:00 EB 301

Optical properties of pyrochlore iridates: signatures of electron correlation and spin-orbit-lattice coupling — •Alexander Boris[1], Alexander Yaresko[1], Timofei Larkin[1], Ksenia Rabinovich[1], Aleksandra Krajewska[1,2], Tomohiro Takayama[1,2], Hidenori Takagi[1,2], and Bernhard Keimer[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]University of Stuttgart, Stuttgart, Germany

Spectroscopic ellipsometry is used to determine the dielectric function of $A_2Ir_2O_7$ (A = In, Lu, Y) polycrystalline samples in the wide spectral range from 10 meV to 6.5 eV at temperatures from 7 K to 300 K. Comparing the spectra with the results of relativistic LSDA+U band structure calculations, we quantitatively classify pyrochlore $A_2Ir_2O_7$ as spin-orbital $J_{eff} = 1/2$ Mott insulators with the on-site Coulomb interaction $U \approx 1.5$ eV and electronic bandwidths $W = 0.3 \div 0.5$ eV. Exciton doublets with pronounced Fano line shapes were identified in $Y_2Ir_2O_7$ and $Lu_2Ir_2O_7$ upon cooling below the magnetic ordering temperatures $T_N = 150$ K and 145 K, respectively. Our results indicate considerable effects of long-range Coulomb interaction and spin-orbit-lattice coupling in the 5d pyrochlore compounds and the need for a detailed analysis of their influence on the $J_{eff} = 1/2$ states. Newly synthesized $In_2Ir_2O_7$ does not exhibit the absorption edge and phonon anomalies below $T_N = 45$ K and thus serves as a reference.

MA 5.11 Mon 12:15 EB 301

Anisotropy of the spin-fluctuations and its impact on the symmetry of the order parameter in the unconventional Sr2RuO4 superconductor. — S. Khmelevskyi[1], B. Kim[2], D. D. F. Agterberg[3], P. Mohn[1], •I. I. Mazin[4], and C. Franchini[2] — [1]Center for Computational Materials Science, Vienna University of Technology, Vienna, Austria — [2]Center for Computational Materials Physics, Vienna University, Vienna, Austria — [3]University of Wisconsin, Milwaukee, USA. — [4]Naval Research Laboratory, Washington DC, USA.

The superconductivity (SC) in the Sr2RuO4 has attracted a considerable interest in the past two decades comparable to that in cuprates and iron pnictides. NMR experiments strongly suggested a triplet chiral order parameter, while more recent probes of strained crystals point toward singlet pairing. In this work the structure of the spin-fluctuations in the Sr2RuO4 has been investigated from first principles using the DLM formalism and Lichtenstein method. We find that IC spin-fluctuations are stabilized but several magnetic ground states with q close to the commensurate (1/3, 1/3, 0) value are degenerate. We show that the degeneration is removed by Spin-orbit coupling and a very special collinear modulated magnetic structure with periodicity 1/3 is stabilized in the mean field in the [110] direction. We show that anisotropic magnetic terms provide an energy penalty for rotating the order parameter that is several orders of magnitude too large for the accepted interpretation, thus rendering the NMR experiment completely inexplicable in terms of the conventional theory.

MA 5.12 Mon 12:30 EB 301

Magnetic shape-memory effect in $SrRuO_3$ — •Daniel Brüning[1], Stefan Kunkemöller[1], Agung Nugroho[2], Isabelle Stunault[3], Markus Braden[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Faculty of Mathematics and Natural Science, Institut Teknologi Bandung, Indonesia — [3]Institut Laue Langevin, Grenoble, France

As most perovskites, $SrRuO_3$ exhibits structural phase transitions associated with rotations of the RuO_6 octahedra. From a high temperature cubic phase it becomes tetragonal at 975 K and orthorhombic at 800 K resulting in six possible domains. Furthermore, $SrRuO_3$ orders ferromagnetically at $T_c = 160$ K with easy axis anisotropy due to spin orbit coupling. Our neutron diffraction and macroscopic measurements unambiguously show that magnetic fields rearrange structural domains, although the ferromagnetic order occurs at six times lower temperature than the structural distortion. For the field along a cubic $[110]_c$ direction, a fully detwinned crystal is obtained. Subsequent heating above T_c causes a magnetic shape-memory effect, where the initial structural domains recover, which is similar to Heusler alloys.

Kunkemöller *et al.*, arXiv:1709.05688 (2017)
Funded by the DFG via CRC 1238 Projects A02, B01, and B04.

MA 5.13 Mon 12:45 EB 301

Multicritical Lifshitz transition of the Fermi-surface in $Sr_3Ru_2O_7$ — •Joseph Betouras[1], Dmitry Efremov[1,2], Alex Shtyk[3], Andreas Rost[4], Claudio Chamon[5], and Andrew Mackenzie[4,6] — [1]Department of Physics, Loughborough University, Loughborough, UK — [2]Leibniz-Institut fur Festkorper- und Werkstoffforschung, D-01069 Dresden, Germany — [3]Department of Physics, Harvard University, Cambridge, MA 02138, USA — [4]SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, U.K. — [5]Department of Physics, Boston University, Boston, MA, 02215, USA — [6]Max Planck Institute for Chemical Physics of Solids, Noethnitzer Str. 40, 01187 Dresden, Germany

We present a theoretical framework, supported by experimental evidence for a Lifshitz topological transition of the Fermi surface in the ultra-clean layered perovskite metal $Sr_3Ru_2O_7$ [1]. Strong power-law dependence of the density of states on energy, associated to the topological transition, in addition to other main features of the Fermi surface as well as interactions, can lead to novel physics. As a consequence, many yet unexplained properties of the thermodynamics and formation of phases of this material can be understood. In particular, we naturally explain the increase of the entropy[2] as well as the formation of spin density wave (phase A) [3]. This work provides an example of the power of Fermi surface topological transitions.

[1]S. A. Grigera, S. A. et al. Science 306, 1154 (2004).
[2] A. Rost et al., Science 325, 1360 (2009).
[3] C. Lester et al, Nature Materials 14, 373 (2014).

MA 5.14 Mon 13:00 EB 301

Study of reorientation in $NdFe_{0.5}Mn_{0.5}O_3$ — Ankita Singh[1], Anil Jain[2], Avijeet Ray[1], Vivian Nassif[3], Tulika Maitra[1], and •Vivek K. Malik[1] — [1]Department of Physics, IIT Roorkee, Roorkee, 247667, India — [2]Solid State Physics Division, Bhabha Atomic Research Center, Mumbai 400085, India — [3]Institut Laue -Langevin, 71 Avenue des Martyrs, 38000 Grenoble, cedex 9 France

In the present study, we have studied spin reorientation in $NdFe_{0.5}Mn_{0.5}O_3$ using neutron powder diffraction technique. Polycrystalline compound $NdFe_{0.5}Mn_{0.5}O_3$ was synthesized using the standard solid state reaction method. Neutron powder diffraction experiments over the temperature range of 1.5-300 K have been performed. Our neutron diffraction study shows that below the Néel temperature (T_N250 K), the magnetic structure (for the Fe/Mn spins) is a G-type antiferromagnet [corresponding to the Γ_1 representation with spins aligned along the crystallographic b direction. Below 70 K, additional peaks appear in the neutron diffraction pattern. Rietveld refinement (below 70 K) confirms a coexistence of two magnetic phases corresponding to representations Γ_1 and Γ_2. In the magnetic structure corresponding to the Γ_2 representation, Fe/Mn spins are aligned along the crystallographic c direction (with small ferromagnetic component along the crystallographic a axis). Upon cooling (below 50 K), the phase fraction of the second magnetic phase increases. At 1.5 K, magnetic structure can be described only by Γ_2 representation. An antisymmetric exchange interaction between R^{3+}-Mn^{3+}/Fe^{3+}spins might be responsible for the observed spin reorientation.