MA 42: Magnetic Materials III

Time: Thursday 15:00–18:15 Location: HSZ 04

MA 42.1 Thu 15:00 HSZ 04

Stabilization of a structural pattern by local magnetic exchange in MnPtSi — Sarah Ackerbauer, •Andreas Leithe-Jasper, Walter Schnelle, Helge Rosner, and Yuri Grin — Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Straße 40, 01187 Dresden

Among the inorganic materials in general and intermetallic compounds in particular, the ternary phases with the stoichiometric ratio 1:1:1 belong to one of the largest families. The Pearson's Crystal Data - Crystal Structure Database for Inorganic Compounds counts several hundreds of the equiatomic phases. Despite a relatively simple component ratio more than 15 structure types have been found for the compounds of this group. This - on the first glance unexpected finding - is directly connected with the mechanisms of chemical bonding in intermetallic compounds. A possible scenarios may be described by two different energy scales: On the larger scale, an atomic arrangement is formed by combination of covalent and ionic interactions in accordance with the electronic needs of constituting elements. The final tuning of the structure is performed at a smaller scale and includes additional atomic interactions. In particular, paramagnetism of the components can be decisive for the achieving of the minimum of the total energy in the second step. The analysis of chemical bonding in MnPtSi reveals that the local magnetism of Mn rules its finally adopted structure.

MA 42.2 Thu 15:15 HSZ 04

Quantum oscillations and high carrier mobility in the delafossites PdCoO2 and PdCrO2 — •Clifford Hicks[1,2], Alexandra Gibbs[1], Andrew Mackenzie[1,2], Hiroshi Takatsu[3,4], Yoshiteru Maeno[4], and Edward Yelland[1] — [1]University of St Andrews, St Andrews, United Kingdom — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]Tokyo Metropolitan University, Tokyo, Japan — [4]Kyoto University, Kyoto, Japan

We present torque magnetometry and resistivity data on single crystals of the delafossites $PdCoO_2$ and $PdCrO_2$. At 295 K we measure an in-plane resistivity of 2.6 $\mu\Omega$-cm in $PdCoO_2$, making it the most conductive oxide known. $PdCrO_2$ has the same crystal structure as $PdCoO_2$, but is a triangular antiferromagnetic metal. Apart from the addition of the magnetism, the electronic structure of $PdCrO_2$ is strikingly similar to that of $PdCoO_2$, and comparison of these two metals provides an opportunity to isolate the effects of the magnetism.

MA 42.3 Thu 15:30 HSZ 04

Angle-resolved photoemission spectroscopy on iron-chalcogenide superconductors — •Janek Maletz[1], Volodymyr Zabolotnyy[1], Daniil Evtushinsky[1], Setti Thirupathaiah[1], Anja Wolter-Giraud[1], Luminita Harnagea[1], Alexander Yaresko[3], Alexander Vasiliev[4], Dimitri Chareev[5], Emile Rienks[6], Bernd Büchner[1,2], Alexander Kordyuk[1], Zurab Shermadini[7], Hubertus Luetkens[7], Kamil Sedlak[7], Rustem Khasanov[7], Alex Amato[7], Anna Krzton-Maziopa[7], Kazimierz Conder[7], Ekaterina Pomjakushina[7], Hans-Henning Klauss[2], and Sergey Borisenko[1] — [1]IFW Dresden — [2]TU Dresden — [3]MPI-FKF, Stuttgart — [4]Moscow State University — [5]RAS, Chernogolovka, Russia — [6]Helmholtz-Zentrum Berlin — [7]Paul Scherrer Institute, Switzerland

The electronic structure of the iron chalcogenide superconductors $FeSe_{1-x}$ and $Rb_{0.77}Fe_{1.61}Se_2$ was investigated by high-resolution angle-resolved photoemission spectroscopy (ARPES). The results were compared to DFT calculations and μSR measurements. Both compounds share "cigar-shaped" Fermi surface sheets in their electronic structure, that can be found in almost all iron-pnictide superconductors. These features originate from a strong interplay of two hole- and electron-like bands in the Brillouin zone center, leading to a pronounced singularity in the density of states just below the Fermi level. This faciliates the coupling to a bosonic mode responsible for superconductivity. This work was supported by the DFG Schwerpunktprogramm 1458 (BO1912/3-1 and BO1912/2-2).

MA 42.4 Thu 15:45 HSZ 04

Spin-liquid phase and order-by-disorder on the frustrated swedenborgite-lattice — •Stefan Buhrandt[1] and Lars Fritz[2] — [1]Institut für theoretische Physik, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [2]Institute for Theoretical Physics, Utrecht University, Leuvenlaan 4, 3584 CE Utrecht, The Netherlands

The phenomenon of frustration refers to the inability to satisfy competing interactions simultaneously. Often, strong frustration leads to a large number of degenerate ground states with fluctuations suppressing the ordering tendencies. A challenging task is to characterize the spin-liquid phase resulting from the inability to order and the eventual breaking of ground state degeneracy. While this is usually accomplished by small perturbations, an intrinsic effect is entropic order-by-disorder. We present evidence that a classical nearest-neighbor Heisenberg model on the swedenborgite lattice hosts both an extended spin-liquid phase as well as a version of entropic order-by-disorder taking place at very low temperatures. We argue that this observation renders magnetic insulators on the swedenborgite lattice a prime candidate for displaying spin liquid and order-by-disorder physics.

MA 42.5 Thu 16:00 HSZ 04

Long range incommensurable spin ordering in a swedenborgite compound — •Johannes Reim[1], Martin Valldor[2], and Werner Schweika[1] — [1]Jülich Centre for Neutron Science JCNS-2 and Peter Grünberg Institut PGI-4, Forschungszentrum Jülich, Jülich, Germany — [2]II. Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

The new swedenborgite compound family ($P6_3mc$) displays similarly to the pyrochlores a highly frustrated network of tetrahedral coordinated magnetic ions. However, its broken inversion symmetry raises further the complexity of ordering due to non-vanashing DM interactions. Recently investigated materials of this family show various signs for unusual geometric frustration. In compounds with magnetic Co and Fe ions, where single crystals are available like $CaBaCo_2Fe_2O_7$, we observed an antiferromagnetic ordering below $T_N \approx 160\,K$, which, however, turned out to be rather complex. Diffuse neutron scattering at DNS (FRM II) has revealed a magnetic order in a three times larger supercell. A particular intriguing result was the chiral interference observed apparently as an asymmetry of the magnetic Bragg intensities. Further powder diffraction experiments at POWGEN (SNS) with higher resolution evidenced additional satellite peaks close to the main magnetic peaks, with a propagation vector $\tau = 0.016\,\text{Å}^{-1}$ corresponding to a long periodicity of about 400 Å.

15 min. break

MA 42.6 Thu 16:30 HSZ 04

Theoretical investigations on the phase diagram of Cr-Sb and Cr-V-Sb — •Gerhard Kuhn[1], Svitlana Polesya[1], Sergiy Mankovsky[1], Hubert Ebert[1], Matthias Regus[2], and Wolfgang Bensch[2] — [1]Ludwig-Maximilians-Universität München — [2]Christian-Albrechts-Universtität zu Kiel

Investigations on the phase diagram of Cr-Sb, especially Cr_3Sb have been performed, using the Munich KKR package, that combines density functional theory (DFT) with an all electron Green's function (GF) method. Nonstoichiometric systems have been dealt with by means of the coherent potential approximations (CPA). To investigate temperature dependent magnetic properties Monte Carlo (MC) simulations based on the exchange coupling constants J_{ij} calculated by Lichtenstein's formula have been performed.

While the Cr_3Si-structure, that is assumed to be the ground state, is a simple paramagnet, different possible meta-stable structures, especially the Cr_3Sb DO3 phase and the Heusler-like Cr_2VSb phase, show interesting half-metallic behavior. It can be shown, that in both cases the magnetic moments behave according to the Slater-Pauling-rules. Calculations show that the half-metalicity as well as the Slater-Pauling behavior is destroyed for V_2CrSb and V_3Sb. The ferri-magnetic order of the system can be explained by the anti-ferromagnetic interactions between Cr-atoms with different spin. The critical Temperatures T_C have been calculated for different lattice constants. In addition the Gilbert damping parameter have been calculated for the investigated system.

MA 42.7 Thu 16:45 HSZ 04

Small damping parameters in Co_2FeSi and Fe_2CoSi films — •Christian Sterwerf[1], Markus Meinert[1], Jan-Michael Schmalhorst[1], Behrouz Khodadadi[2], Soumalya Paul[2], Matthias

Buchmeier[2], Claudia Mewes[2], Tim Mewes[2], and Günter Reiss[1] — [1]Thin Films and Physics of Nanostructures, Department of Physics, Bielefeld University, 33501 Bielefeld, Germany — [2]Department of Physics and Astronomy/MINT Center, University of Alabama, Tuscaloosa, Alabama 35487, USA

Co and Fe based Heusler compounds are promising candidates for spintronic devices as they offer high Curie temperatues and high spin polarizations.

In an earlier publication we presented sputtered $Co_{2-x}Fe_{1+x}Si$ ($0 \leq x \leq 1$) films with good crystalline ordering and high tunnel magnetoresistance (TMR) ratios in magnetic tunnel junctions (MTJs) with a $Co_{2-x}Fe_{1+x}Si$ electrode. [1]

Magnetization relaxation and the anisotropy of the films were determined by broadband ferromagnetic resonance (FMR) and magnetooptical Kerr effect (MOKE) measurements. With the help of a broadband FMR and the consideration of the extrinsic linewidth, very small damping parameters were found. The damping parameter for Co_2FeSi is 0.002.

[1] Sterwerf, Christian, et al. "High TMR Ratio in Co_2FeSi and Fe_2CoSi based Magnetic Tunnel Junctions." *IEEE Transactions on Magnetics* 49.7 (2013): 4386.

MA 42.8 Thu 17:00 HSZ 04

Element resolved atomic vibrational properties of magnetocaloric $LaFe_{13-x}Si_x$ — •Markus Ernst Gruner[1,2], Werner Keune[2,3], Beatriz Roldan Cuenya[4], Joachim Landers[2], Sergey Makarov[2], David Klar[2], Michael Y. Hu[5], Ercan E. Alp[5], Maria Krautz[1], Oliver Gutfleisch[6], and Heiko Wende[2] — [1]IFW Dresden — [2]Universität Duisburg-Essen — [3]MPI Halle — [4]Ruhr-Universität Bochum — [5]Argonne National Laboratory — [6]TU Darmstadt

Large magnetocaloric effects are obtained at discontinuous magnetic phase transitions, which are preferentially close to second-order as this keeps hysteresis losses small. In $LaFe_{13-x}Si_x$, the first order character is connected with a significant volume decrease upon disordering the magnetic subsystem, arising from the coupling of magnetic and elastic degrees of freedom. Their contribution to the total entropy change is thus not necessarily cooperative. By comparing nuclear resonant inelastic X-ray scattering (NRIXS) with a sample with 10 % ^{57}Fe isotopic enrichment ($x = 1.4$) and extensive DFT modeling ($x = 1.5$) we obtain the element and site-resolved phonon density of states in the ordered and the paramagnetic state. These allow us to understand the impact of magnetoelastic interactions on the vibrational entropy change at the magnetic phase transition.

MA 42.9 Thu 17:15 HSZ 04

Study of the magnetocaloric effect in MnFe4Si3 — •Paul Hering[1], Karen Friese[1], Jörg Voigt[1], Thomas Brückel[1], Anatoliy Senyshyn[2], Nadir Aliouane[2,3], and Andrzej Grzechnik[4] — [1]JCNS-2/PGI 4, Forschungszentrum Jülich — [2]MLZ, TUM, Garching — [3]PSI, Villigen, Schweiz — [4]Inst. of Crystallo., RWTH Aachen

Due to global warming, there is an increasing demand for more energy-efficient refrigeration technologies. Magnetocaloric devices are candidates to replace conventional vapor compression cooling, as they have potentially 20-30% lower energy consumption. MnFe4Si3 is a promising candidate for magnetic cooling at ambient temperatures [Songlin, et. al., J. Alloys Comp. 334, 249 (2002)]. To understand the interplay of the spin and lattice degrees of freedom in this material, we studied the magnetic properties and the temperature dependent evolution of its hexagonal structure. The compound undergoes a magnetic phase transition close to 300K, which is accompanied by a modestly high magnetocaloric effect (MCE) of 2.9 J/kg K at a magnetic field change from 0T to 2T. Refinements with the program Jana2006 using single crystal neutron and x-ray data simultaneously show that in the ferromagnetically ordered structure the magnetic moments are aligned in the a,b-plane. Magnetic susceptibility measurements confirm the easy axis of magnetization perpendicular to the c-axis. Lattice parameter obtained from neutron powder diffraction data show a discontinuous change at the temperature of the onset of magnetic ordering. This clearly indicates the first order character of the phase transition and explains the relatively high MCE.

MA 42.10 Thu 17:30 HSZ 04

Direct measurement of the magnetocaloric effect in $La(Fe,Si,Co)_{13}$ compounds in pulsed magnetic fields — •M. Ghorbani[1,2], Y. Skourski[1], K.P. Skokov[3], M.D. Kuz'min[3], O. Gutfleisch[3], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD), Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden — [2]Institut für Festkörperphysik, TU Dresden, 01069 Dresden, Germany — [3]Institut für Materialwissenschaft, TU Darmstadt, Germany

We report on direct measurements of the magnetocaloric effect (MCE) of $La(Fe,Si,Co)_{13}$ compounds, which are promising candidates for magnetic refrigeration applications as they undergo a metamagnetic transition associated with substantial entropy change. The nature of the transition can be changed from first to second order. Further, the temperature of the transition is tunable by varying the Co concentration. We have measured the MCE for two compounds with different Co concentrations with transition temperatures of 199 K (first order) and 254 K (second order). At low fields the former compound shows a higher MCE, but at the maximum field of 50 Tesla both compounds yield similar temperature changes of about 15 K.

MA 42.11 Thu 17:45 HSZ 04

Magnetic and magnetocaloric properties of the MnB system — •Maximilian Fries, Konstantin Skokov, and Oliver Gutfleisch — TU Darmstadt, Materialwissenschaften, 64287 Darmstadt

Magnetocalorics is a thriving research topic and materials that exhibit this effect become of high demand in case magnetic cooling can one day replace conventional refrigeration technologies. Especially materials with critical elements like rare earths, for example the reference material Gadolinium, are relevant in this field. To overcome this problem a lot of research is focused on finding materials which exhibit a magnetic transition (e.g. FM to PM) coupled to a structural transition at the desired transition temperature containing no critical elements. Such developments will reduce both raw material use and future technology cost. Here we report on the magnetic and structural properties of the compound MnB which undergoes a FM to PM transition at about 570K with minimal hysteresis, exhibiting an entropy change of 7 J/kgK in a field change of 0-2T. Furthermore we show results on the substitution in the compound MnxB in order to tune the Curie temperature and the magnetocaloric properties in this material system.

MA 42.12 Thu 18:00 HSZ 04

First-principles simulation of the instability leading to giant magnetocaloric effects — •Peter Entel, Markus Gruner, and Anna Grünebohm — Faculty of Physics and CENIDE, University of Duisburg-Essen, 47048 Duisburg

Ferroic cooling using magnetic solids may lead to a technological breakthrough in future cooling devices. In particular magnetic Heusler alloys such as Ni-Co-Mn-(Ga, In, Sn), and La-Fe-Si, Ga-Mn-C-N and Fe-P based alloys have proven to be suitable for magnetic refrigeration besides the ternary compound Gd-Ge-Si showing giant magnetocaloric effect (MCE). Here, we will address the important aspect of the sudden drop of the magnetization from the ferromagnetic to an antiferromagnetic/paramagnetic state near the magnetostructural transition which is responsible for the giant inverse MCE in some of these systems. We employ density functional theory (DFT) together with finite-temperature Monte Carlo (MC) simulations in the investigations showing that the size of the jump of magnetization in external magnetic fields defines the MCE. Adding elements like Co to the ternary compounds, which is accurately handled in the DFT and MC simulations, allows to explore optimization of the MCE.