MA 3: Magnetic Materials I

Time: Monday 10:15–13:00 Location: H22

MA 3.1 Mon 10:15 H22

Melt-spun MnFe(P,Ge,Si) as a giant magnetocaloric material — •Oliver Gutfleisch, Wei Zhang, Julia Lyubina, and Ludwig Schultz — Leibniz Institute of Solid State and Materials Research Dresden (IFW Dresden), Institute of Metallic Materials, P.O. Box 270016, D-01171 Dresden, Germany

The giant magnetocaloric effect was studied in Mn1.1Fe0.9P0.8-xSixGe0.2 (x=0.1, 0.12, 0.13, 0.14) and Mn1.1Fe0.9P0.85-xSixGe0.15 (x=0.18, 0.2, 0.22) melt-spun ribbons. Thermal, structural and magnetic properties were investigated by SQUID, PPMS, XRD and SEM. The dependence of Curie-temperature, thermal and magnetic hysteresis, crystal lattice parameters and magnetic entropy changes on composition are described. It is demonstrated that melt-spinning [1,2] is a efficient and very simple processing route for MnFe(P,Ge,Si)-type materials, i.e. arsenic free Fe2P-type alloys [3], exhibiting large values of magnetic entropy change (|deltaS(m)|=45J/kgK) with very small magnetic hysteresis near room temperature.

[1] O. Gutfleisch et al., J. Appl. Phys. 97 (2005) 10M305. [2] A. Yan, et al., J. Appl. Phys. 99 (2006) 08K903. [3] D.T. Cam Thanh et al., J. Appl. Phys. 99 (2006) 08Q107.

MA 3.2 Mon 10:30 H22

Investigation of $Rb_4(O_2)_3$, a predicted Halfmetallic Ferromagnet — •Jürgen Winterlik[1], Gerhard H. Fecher[1], Claudia Felser[1], Martin Jansen[2], Claus Muehle[2], and Franziska Emmerling[3] — [1]Johannes-Gutenberg-Universität Mainz — [2]MPI Stuttgart — [3]BAM Berlin

The black colour of Rubidium Sesquioxide $Rb_4(O_2)_3$, an alkali oxide containing two superoxide anions and one peroxide anion, indicates an exceptional electronic structure compared to similar substances. Band structure calculations gave advice that $Rb_4(O_2)_3$ might be an anionogenic halfmetallic ferromagnet with magnetism based on oxygen-2p-electrons.

Neutron diffraction measurements reveal that the substance crystallises in the cubic space group I-43d. Magnetic measurements of the substance, performed by SQUID magnetometry, show dominating antiferromagnetic interactions with indications of a frustrated system due to thermal hysteresis and lack of saturation. An effective moment of 1.95 μ_B matches the expected value of 2 μ_B quite well. The experimental data are compared to electronic structure calculations.

MA 3.3 Mon 10:45 H22

Non-adiabatic spin dynamics in thin magnetic films — •Pawel Buczek, Arthur Ernst, Leonid Sandratskii, and Patrick Bruno — Max Planck Institute of Microstructure Physics

The thermal properties of magnetic materials are essentially influenced by the spectrum of spin fluctuations (magnons and Stoner excitations), both in bulk materials and in the systems with reduced dimensionality, e.g. films.

For small wave-length excitations, it is crucial to treat both the magnons and Stoner excitations dynamically, on an equal footing, especially in systems with reduced dimensionality. The most reliable way to consider magnon properties is by the computation of frequency-dependent magnetic susceptibility.

In our project the ground state of a magnetic film is generated by means of layered KKR Green's function method. Subsequently, the magnetic susceptibility is constructed in a two-step procedure. First, an auto-convolution of the KKR Green's function (non-enhanced susceptibility) is constructed. In the next step, true susceptibility is obtained through a solution of a selfconsistent integral equation, originating from the time dependent DFT. Layered KKR has the advantage of yielding realistic band structure; also the relaxations of the film crystalline structure in the direction perpendicular to its surface can be taken into account.

In the presentation the fundamentals of the method will be discussed along with several preliminary results on magnetic excitations in bulk Fe and its thin films.

MA 3.4 Mon 11:00 H22

Bestimmung der Ordnungsparameter in epitaktischen Fe_3Si-Filmen auf MgO(001) mittels Mössbauerspektroskopie — •Natalia Utochkina[1], Marco Walterfang[2], Werner Keune[1] und Heiko Wende[1] — [1]Fachbereich Physik, Universität Duisburg-Essen, D-47048 Duisburg — [2]ACCESS e.V. Materials & Processes, D-52072 Aachen

Fe_3Si-Legierungen sind aufgrund ihrer hohen Spinpolarisation für das sich schnell entwickelnde neue Gebiet der Spinelektronik und Magnetoelektronik interessant geworden. Epitaktische Fe_3Si-Filme auf MgO(001) wurden durch Koverdampfen im UHV bei verschiedenen Wachstums- (T_S-) und Anlass- (T_A-) Temperaturen präpariert und mittels Röntgenbeugung untersucht. Es wurde eine Gitterplatz-Besetzungsanalyse von Fe-Atomen mittels ^{57}Fe-CEMS durchgeführt. Die atomaren Nachbarkonfigurationen und Nahordnungsparameter α_1 und α_2 ergaben sich aus der Analyse der verschiedenen spektralen Sextett-Komponenten hinsichtlich magnetischem Hyperfeinfeld und relativer Intensität. Um die langreichweitigen Ordnungsparameter S zu bestimmen, wurden mittels Computersimulation willkürliche Abweichungen von der idealen $D0_3$-Struktur bei 25 at.% Si und dadurch gewünschte Werte der Si-Konzentration und des Ordnungsgrades erzeugt. Der Vergleich der Simulation mit den Mössbauer-Resultaten ergab die Ordungsparameter S($D0_3$) und S(B2). Die höchste Ordnung (α_1=-0.33, α_2=-0.32, S(D03)=0.99, S(B2)=0.66) wurde bei T_S=250 °C und T_A=600 °C beobachtet.

Gefördert durch die DFG (SFB 491).

MA 3.5 Mon 11:15 H22

Interfacial features of $La_{0.7}Sr_{0.3}MnO_3$ probed by scanning tunneling microscopy — •Lakshamana Sudheendra, Markus Esseling, Vasily Moshnyaga, Bernd Damaschke, and Konrad Samwer — I. Physikalisches Insitut, Friedrich-Hund-Platz-1, 37077, Göttingen, Germany

We present scanning tunneling microscopy (STM) and spectroscopy (STS) studies on artificial grain boundary (GB) resulting from the growth of Sr-substituted manganite on MgO bicrystal substrate. The width of the GB-the region between the two crystals- was found to be around 20-30 nm, wherein unusual structural and electronic features were observed in the topography and spectroscopy. Within the GB, structural features running parallel to the grain boundary were detected, which originate probably due to relaxation of stress. Tunneling conductivity within the GB at room temperature was found to be insulating-like, and could be strongly increased through the interaction between the tip and film. The puzzle of sharp [1] versus diffused [2] electronic phase separation between two different electronic phases appears to be linked to domains/antiphase boundaries versus disorder/strain.

[1]. Ch. Renner et al., Nature, 416, 518 (2002).
[2]. T. Becker et al., Phys. Rev. Lett. 89, 237203 (2002).

Acknowledgement: We acknowledge the support of DFG-SFB 602 TP A2 and the Leibniz program.

MA 3.6 Mon 11:30 H22

Bulk sensitive photo emission spectroscopy of $C1_b$ compounds — •Benjamin Balke[1], Gerhard H. Fecher[1], Andrei Gloskovskii[1], Joachim Barth[1], Claudia Felser[1], Franz Schäfers[2], Marcel Mertin[2], Wolfgang Eberhardt[2], Sven Mähl[3], and Oliver Schaff[3] — [1]Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg - Universität Mainz, Germany — [2]BESSY GmbH, Albert-Einstein-Straße 15, 12489 Berlin, Germany — [3]SPECS GmbH, Voltastraße 5, 13355 Berlin, Germany

This work reports about bulk-sensitive, high energy photoelectron spectroscopy from the valence band of CoTiSb excited by photons from 1.2 to 5 keV energy. The high energy photoelectron spectra were taken at the KMC-1 high energy beamline of BESSY II employing the recently developed Phoibos 225 HV analyser. The measurements show a good agreement to calculations of the electronic structure using the LDA scheme. It is shown that the high energy spectra reveal the bulk electronic structure better compared to low energy XPS spectra.

MA 3.7 Mon 11:45 H22

Magnetic order in highly oriented graphite irradiated with protons at low temperatures — •Jose Barzola-Quiquia[1], Martin Rothermel[2], Annette Setzer[1], Pablo Esquinazi[1], and Tilman Butz[2] — [1]Division of Superconductivity and Magnetism, Institute for Experimental Physics II, University of Leipzig, Linnéstr. 5, 04103

Leipzig, Germany — [2]Division of Nuclear Solid State Physics, Institute for Experimental Physics II, University of Leipzig, Linnéstrasse 5, 04103 Leipzig, Germany

In this contribution we compare the magnetic properties of graphite samples proton irradiated at room and low (T=110K) temperatures. An array of 160x160 spots of micrometer size were proton irradiated with fluence of $\sim$1nC/μm^2 in highly oriented graphite samples, two of them at low and one at room temperature. Special sample holders, which enable irradiation and SQUID measurements without any sample handling, allow us to study with high accuracy the changes produced by the irradiation on the magnetic properties. SQUID measurements reveal clear differences between the low and room temperatures irradiations. The samples irradiated at low temperature show larger ferromagnetic contribution. From the temperature dependence of the ferromagnetic contribution we obtain a Curie temperature of the order of 400K for the micrometer size irradiated spots. The total amount of magnetic impurities, measured in situ and during irradiation, is below 0.3 ppm and cannot explain the observed magnetic order. Our results confirmed previous results published earlier in Phys..Rev.Lett. **91**, 227201 (2003).

MA 3.8 Mon 12:00 H22

Bulk and surface magnetism in $Na_{0.75}CoO2$: why is Luttinger's theorem violated? — •Michelle Johannes[1], Igor Mazin[1], and George Sawatzky[2] — [1]Naval Research Laboratory, Washington, D.C. USA — [2]University of British Columbia, Vancouver, Canada

The properties of Na_xCoO_2 vary substantially with the sodium concentration, x. Though strong spin fluctuations are proposed to exist throughout the full range of sodium, long range magnetic order sets in only at low hole concentration (x $\sim$ 0.7). Also around this doping, ARPES results show substantial disagreement with Luttinger's theorem (LT). We show that this is definitively not the result of deviations from two-dimensionality and propose that the two effects (magnetism and violation of LT) are related. We present a careful analysis of the various possible terminations of a cleaved surface of $Na_{0.75}CoO_2$, and conclude that the observed Fermi surfaces are inconsistent with ANY physically possible bulk system. We suggest surface layer magnetism as a possible explanation for the discrepancy between Fermi surface size and electron count.

MA 3.9 Mon 12:15 H22

Unexpectedly Strong Magnetic Coupling in Rare Earth Borides — •Takao Mori[1,2] and Yuri Grin[2] — [1]National Institute for Materials Science, Nanoscale Materials Center, Namiki 1-1, Tsukuba, 305-0044, Japan — [2]Max Planck Institute for Chemical Physics of Solids, Noethnitzer Str. 40, 01187 Dresden, Germany

The magnetism of rare earth borides like REB_4, REB_6, and REB_{12} has attracted a lot of interest over the years. These compounds are all good metals in the case of trivalent rare earth elements and their magnetic coupling has basically been described by the Ruderman-Kittel-Kasuya-Yoshida (RKKY) mechanism. As an emerging new phenomenon, it has been found that borides which contain the B_{12} icosahedra as a structural building block can exhibit unexpectedly strong magnetic interactions despite being relatively magnetically dilute insulators (e.g. T_N = 17 K for TbB_{50} and T_f = 29 K for $HoB_{17}CN$) [1-3]. We report on a new phase discovered in a series of homologous rare earth boron carbonitride compounds which have a particular triangular configuration of the rare earth atoms. The dynamical properties investigation of $HoB_{22}C_2N$ has previously indicated that it is a two-dimensional spin glass. Magnetic and thermoelectric properties of this series of compounds are presented.

[1] T. Mori and T. Tanaka, J. Phys. Soc. Jpn. **68** 2033 (1999). [2] T. Mori and H. Mamiya, Phys. Rev. B **68**, 214422 (2003). [3] T. Mori, J. Appl. Phys. **95**, 7204 (2004).

MA 3.10 Mon 12:30 H22

The antiferromagnetic ground state on 2D kagomé lattices in Y0.5Ca0.5BaCo4O7 — •Martin Valldor[1] and Werner Schweika[2] — [1]II. Phys. Inst., Zülpicher Str. 77, D-50937 Köln — [2]Institut für Festkörperforschung, FZ Jülich, D-52425 Jülich

The compound Y0.5Ca0.5BaCo4O7 contains a net of tetrahedrally coordinated Co, similar to that in the wurtzite type structure. The transition metal sublattice forms perfect kagomé type layers and the intralayer coupling is much stronger than any inter-layer interaction, giving low-dimensional magnetism. Frustration and an unusual spin state of the inter-layers Co cause the layers to magnetically decouple. The susceptibility measurements indicate strong antiferromagnetic coupling between spins [1], but the magnetic part of neutron diffraction data, separated through polarization, shows no long-range order down to 1.2 K [2]. The observed diffuse peak indicates an ordering tendency towards a staggered chiral ground state, a spin structure of Heisenberg spins in layers called V3xV3. This coplanar spin structure exhibits a degeneracy with local chiral disorder even at very low temperatures. Studies of this complex, highly frustrated magnetic state give clues to unique spin ordering effects close to their ground state.

[1] M.Valldor Solid State Sciences 8 (2006) 1272-1280
[2] W.Schweika, M.Valldor, P. Lemmens submitted to PRL (2006)

MA 3.11 Mon 12:45 H22

High-temperature magnetic order in an aromatic polyimide — Jose Barzola-Quiquia[1], •Pablo Esquinazi[1], Annette Setzer[1], Michael Ziese[1], Martin Rothermel[2], Daniel Spemann[2], and Tilman Butz[2] — [1]Division of Superconductivity and Magnetism, Institute for Experimental Physics II, University of Leipzig, Linnéstr. 5, 04103 Leipzig, Germany — [2]Division of Nuclear Solid State Physics, Institute for Experimental Physics II, University of Leipzig, Linnéstr. 5, 04103 Leipzig, Germany

We have studied the temperature and magnetic field dependence of the magnetization of polyimide foils in the as-received state, after annealing at temperatures $T \leq 1000$C and after proton irradiation. The temperature and field dependence depend strongly on the sample initial, annealing as well as on the irradiation conditions. Added to a diamagnetic signal our results provide clear evidence for ferromagnetism and paramagnetism due to different multiplets contributions. The very low magnetic impurity concentration (below 0.5ppm) cannot explain the observed behavior as well as the ferromagnetic and paramagnetic values. The Curie temperature of the ferromagnetic contribution reaches values of the order 800 K upon annealing. The overall results indicate that metal-free polyimides are interesting objects for basic research with potential applications in the area of magnetism.