MA 4 Magnetic Materials I

Time: Monday 10:15–12:45 Room: HSZ 401

MA 4.1 Mon 10:15 HSZ 401

Observation of two ferromagnetic phases in Co-doped rutile TiO_2 — •A. Nefedov[1], N. Akdogan[1], A Westphalen[1], R. Khaibullin[2], L. Tagirov[2], and H. Zabel[1] — [1]Institut für Experimentalphysik/Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany — [2]Kazan Physical-Technical Institute of RAS, 420029 Kazan, Russia

Oxide based diluted magnetic semiconductors have recently attracted considerable attention because of reports of room temperature ferromagnetism in several systems and their projected potential for spintronic devices. However, subsequent reports have raised concerns about the initially suggested intrinsic nature of ferromagnetism in this material.

The magnetic properties of Co-doped TiO_2 synthesized by ion implantation with different implantation doses have been studied using MOKE, SQUID and XRMS methods. We observe paramagnetic behaviour for low dose doped sample, but obtain clear ferromagnetic behaviour for intermediate and high dose doped samples. The drastical change of the hysteresis loop shape at the transition from the intermediate to high Coimplantation doses, demonstrating a presence of 2 ferromagnetic phases in Co-doped rutile TiO_2, has been observed. Origin of these 2 phases will be discussed during the talk.

This work was partially supported by DFG through SFB 491 and by RFBR through grant no. 04-02-97505. N Akdogan acknowledges a fellowship through the Max-Planck Research School "SurMat".

MA 4.2 Mon 10:30 HSZ 401

Correlation in the transition metal based Heusler compounds Co_2MnSi and Co_2FeSi — •Hem Chandra Kandpal, Gerhard H. Fecher, and Claudia Felser — Johannes Gutenberg - Universität, 55099 Mainz, Germany

Half-metallic ferromagnets like the full Heusler compounds are supposed to show an integer value of the magnetic moment. Calculations reveal for Co_2FeSi a non-integer value, in contrast to experiments. In order to explain deviations of the calculated magnetic moment, the dependency of the electronic structure on the lattice parameter was studied theoretically. In LSDA, the minimum total energy of Co_2FeSi is found for the experimental lattice parameter, but the calculated magnetic moment is about 12% too low. Half-metallic ferromagnetism and a magnetic moment equal to the experimental value of $6\mu_B$ are found, however, only after increasing the lattice parameter by more than 6%.

To overcome this discrepancy, the LDA+U scheme was used to include electron correlation in the calculations. The calculations revealed that an effective Coulomb-exchange interaction $U_{eff} = U - J$ in the range of about 2eV to 5eV leads to half-metallic ferromagnetism and the measured, integer magnetic moment at the measured lattice parameter. Finally, it is shown in the case of Co_2MnSi that correlation may also serve to destroy the half-metallic behaviour if it becomes too strong (for Co_2MnSi above 2eV and for Co_2FeSi above 5eV). These findings indicate that on-site correlation may play an important role in the description of Heusler compounds with localized moments. (This work is funded by the DFG in FG 559.)

MA 4.3 Mon 10:45 HSZ 401

Structural and physical properties of the quarternary Heusler alloys $Co_2Mn_{1-x}Fe_xSi$: A search for the optimal material for spintronic devices — •Benjamin Balke, Hem Chandra Kandpal, Vadim Ksenofontov, Gerhard H. Fecher, and Claudia Felser — Johannes Gutenberg - Universität, 55099 Mainz, Germany

The strucural and magnetic properties of the quarternary Heusler alloys $Co_2Mn_{1-x}Fe_xSi$ ($x = 0, 0.1, \ldots, 1$) were investigated by means of X-ray diffraction, SQUID magnetometry, ESCA, ^{57}Fe Mößbauer spectroscopy, and differential scanning calometry messurments. The pure Co_2MnSi compound is allready used as an electrode in magnetic tunnel juctions. Previous LSDA calculations predicted Co_2MnSi to be a half-metallic ferromagnet with a spinpolarisation of 100%, a value that could not be verified by experiments up to now. Recent investigations of the electronic strucutre of Heusler compounds gave advice that on-site correlation plays a role in these componds and may serve to destroy the half-metallic properties of Co_2MnSi. At the same time Co_2FeSi becomes a half-metallic ferromagnet if on-site correlation is respected in electronic structure calculations.

This investigation focuses on the search of a mixed compond where the half-metallic behaviour is stable against the variation of on-site correlation. (This work is funded by the DFG in FG 559.)

MA 4.4 Mon 11:00 HSZ 401

Structural properties of the quaternary Heusler alloy $Co_2Cr_{1-x}Fe_xAl$. — •Jonder Morais[1], Sabine Wurmehl[2], Maria do Carmo M. Alves[1], Sergio R. Teixeira[1], Giovanna Machado[1], Vadim Ksenofontov[2], Gerhard H. Fecher[2], and Claudia Felser[2] — [1]Universidade Federal do Rio Grande do Sul, 91501-970 Porto Alegre, Brazil — [2]Johannes Gutenberg - Universität, 55099 Mainz, Germany

The structural and chemical properties of the Heusler alloy $Co_2Cr_{1-x}Fe_xAl$ (x=0, 0.4, and 1) were investigated comparing powder and bulk samples. The long range order was determined by means of X-ray diffraction and neutron diffraction, while the site specific (short range) order was proved by the extended X-ray absorption fine structure method (EXAFS). The magnetic structure was determined by means of ^{57}Fe Mößbauer spectroscopy in transmission mode as well as in X-ray scattering mode in order to compare powder and bulk properties. The chemical composition was analysed by means of X-ray photo emission spectroscopy (XPS) combined with Auger electron spectroscopy (AES) depth profiling. The results from these methods are compared explain the differences between surface and bulk properties and the appearance of disorder in such alloys. (This work is funded by the DFG in FG 559.)

MA 4.5 Mon 11:15 HSZ 401

Bulk sensitive photoemission spectroscopy of the quaternary Heusler alloy $Co_2Cr_{0.6}Fe_{0.4}Al$. — •Sabine Wurmehl[1], Gerhard H. Fecher[1], Kristian Kroth[1], Florian Kronast[2], Hermann A. Dürr[2], Yukiharu Takeda[3], Yuji Saitoh[3], Keisuke Kobayashi[3,4], Gerd Schönhense[1], and Claudia Felser[1] — [1]Johannes Gutenberg-Universität, 55099 Mainz, Germany — [2]BESSY, 12489 Berlin, Germany — [3]Spring-8 / JAERI, Hyogo, 679-5198, Japan — [4]Spring-8 / JASRI, Hyogo, 679-5198, Japan

Quaternary Heusler alloy $Co_2Cr_{0.6}Fe_{0.4}Al$ was investigated experimentally and theoretically. The electronic structure and spectroscopic properties were calculated using the full relativistic Korringa-Kohn-Rostocker method with coherent potential approximation to account for the random distribution of Cr and Fe atoms as well as random disorder.

Resonant (560eV - 800eV) soft X-ray as well as high resolution - high energy (3.5keV, 8keV) hard X-ray photoemission was used to probe the density of the occupied states in $Co_2Cr_{0.6}Fe_{0.4}Al$. It was found by resonant and high energy photoemission that there is a discrepancy between the experimentally observed and the theoretically calculated density of states in $Co_2Cr_{0.6}Fe_{0.4}Al$. This observation suggests the presence of correlation in Heusler compounds being not accounted for by local (spin) density approximation in its current form. Moreover, strong differences in surface and bulk photoemission spectra reveal the loss of the bulk and structure signature if emission takes mainly place from the surface layer. (This work is funded by the DFG in FG 559.)

MA 4.6 Mon 11:30 HSZ 401

Directional solidification of Ni48Mn30Ga22 — •Martin Pötschke, Uwe Gaitzsch, Stefan Roth, Bernd Rellinghaus, and Ludwig Schultz — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

NiMnGa alloys are among the most intensively studied magnetic shape memory (MSM) materials. The MSM effect is caused by the movement of twin boundaries in a magnetic field. So far, this effect has only been observed in single crystals. The preparation of single crystals, however, is a long time process and thus expensive, and compositional changes along the crystal axis may arise.To expand the MSM effect to polycrystals, directional solidification was applied in order to prepare coarse grained, textured samples. The technique of stationary casting in a preheated ceramic mold mounted on a copper plate was chosen to provide a heat flow towards the bottom of the mold and therefore a directional solidification in the opposite direction. In order to allow for a direct investigation of the resulting microstructure by EBSD measurements, an alloy composition with a martensitic transformation temperature below room temperature was chosen. The transformation temperature was checked by DSC. The preferred growth direction was determined by EBSD.

MA 4.7 Mon 11:45 HSZ 401

Magnetic switching by twin boundary motion in NiMnGa shape memory ferromagnets — •Uwe Gaitzsch, Martin Pötschke, Stefan Roth, Bernd Rellinghaus, and Ludwig Schultz — IFW Dresden, P.O. Box 270116, 01171 Dresden

Magnetic shape memory materials gained a large research interest owing to their capability to deform by some percent via twin boundary motion under the influence of a magnetic field. Concurrently, they are supposed to react faster than conventional shape memory materials because neither heating nor cooling are involved. In our case off-stoichiometric Ni5Mn3Ga2 is used to produce a polycrystalline textured samples. Upon cooling this alloy transforms to a martensitic state at roughly 100°C. The evolving martensitic structure is either orthorhombic or tetragonal and depends on the thermomechanical history of the sample. Since only one of the two possible structures is suitable of providing the mandatory highly moblile twin boundaries, it is important to understand and control the phase formation process by appropriate thermal and mechanical treatment. Once the sample is given a suitable structure, samples for magnetomechanical testing are cut and investigated in magnetic fields of up to 0,8 T in compression tests. In this device the strain up to the crystallographic limit of reference samples could be determined.

MA 4.8 Mon 12:00 HSZ 401

Magnetic shape memory effect in the paramagnetic state of $R\mathrm{Cu}_2$ (R = rare earth) — •Sebastian Raasch[1], Mathias Doerr[1], Andreas Kreyssig[1], Michael Loewenhaupt[1], Martin Rotter[2], and Jens-Uwe Hoffmann[3] — [1]Germany, Technische Universität Dresden, Institut für Festkörperphysik — [2]Austria, University of Vienna, Institute for Chemistry — [3]Germany, Hahn-Meitner-Institut Berlin

We like to present $R\mathrm{Cu}_2$ (R = rare earth) as the first magnetic shape memory (msm) alloy with the magnetic anisotropy of rare earth ions as impelling force. Besides $\mathrm{La}_{2-x}\mathrm{Sr}_x\mathrm{CuO}_4$ $R\mathrm{Cu}_2$ is the second known antiferromagnetic msm-compound class. However, magnetic order is not necessary for the msm effect here. Microstructural changes are possible even above magnetic ordering temperature because the magnetic anisotropy is effective also in the paramagnetic state. $R\mathrm{Cu}_2$ compounds have a pseudohexagonal orthorhombic structure which leads to the fact of three twin variants, each rotated about 60 deg to the others along the pseudohexagonal b axis. To our knowledge $R\mathrm{Cu}_2$ compounds exist exclusively in the martensitic pseudohexagonal state. To move the twin boundaries, a magnetic field of about 3.2 T and a temperature of typical 30 K is necessary. This moving of twin boundaries correlates with magnetostriction measurements, showing a typical length change of two percent. Depending on the field direction a certain twin variant is favored. We will present neutron data from $\mathrm{Tb}_{0.5}\mathrm{Dy}_{0.5}\mathrm{Cu}_2$ confirming a change of the volume fraction of the three twin-variants. The combination of rare earth magnetizm with the msm effect defines a promising field of science.

MA 4.9 Mon 12:15 HSZ 401

NiMnGa fibres for use in polymer composites — •Nils Scheerbaum, Dietrich Hinz, Oliver Gutfleisch, and Ludwig Schultz — IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany

Composites made of polymer and magnetic shape memory particles (MSM particles) may be used as actuators or as mechanical energy absorber for damping applications. Ideally, the MSM particles should be, at the operating temperatures, in the martensitic state and single-crystalline when in the austenitic state. Fibres of 51Ni-27Mn-22Ga (at.%) were prepared by crucible melt extraction. Their size is about 60μm in diameter and 1cm in length. The structural and magnetic properties of the fibres are similar to those of bulk material with the same composition. The grain size of the meltextracted fibres was determined by SEM to about 5μm. In order to achieve grain growth, the fibres were annealed at 1000-1100°C. After annealing, the grain size is in the order of the diameter of the fibres. Also the martensite start and the Curie temperature are affected by the annnealing (varified by DSC and susceptometry). They increase from 30°C to 45°C and from 88°C to 98°C respectively. XRD analyses reveal that the austenite is cubic and that the martensite is tetragonal with the 5M modulation and c/a=0.94. First composites were prepared using different polymers and the fibres applying various magnetic fields to align the MSM particles.

MA 4.10 Mon 12:30 HSZ 401

First-principles investigation of Co wires at Pt(111) step-edges — •Gustav Bihlmayer[1], Stéphanie Baud[2], Christophe Ramseyer[2], and Stefan Blügel[1] — [1]Forschungszentrum Jülich, Institut für Festkörperforschung, Jülich, Germany — [2]Laboratoire de physique moléculaire, UMR CNRS 6624, Besançon, France

We investigate Co wires of different width deposited on step-edges of Pt(111), simulated by a Pt(664) surface. The calculations were preformed within the framework of the density functional theory using the FLAPW method. An adsorbed Co chain showed a magnetic anisotropy energy (MAE) and easy axis in good agreement with experimental data [1]. Inclusion of relaxations turned the easy axis even more in the direction of the upper terrace and quenched the orbital moments and their anisotropy. While this seems unfavorably in comparison to experiment, we argue – based on a decomposition of the contribution to the MAE of the different atoms (Pt or Co) – that relaxations might be an essential part of the calculations including orbital polarizations. We investigated also the evolution of the easy axes and the MAE as function of the number of Co chains deposited on the stepped surface. The results nicely compare to those obtained experimentally [2]. We present a simple model to account for the experimentally observed oscillations of the easy axis.

[1] P.Gambardella et al. Nature 416, p.301 (2002)
[2] P.Gambardella et al. Phys. Rev. Lett. 93 077203 (2004)