MA 9 FV-internes Symposium "Heusler-Legierungen"(Organizers: B. Hillebrands, H. Zabel)

Zeit: Freitag 15:15–18:45 Raum: TU EMH225

Hauptvortrag MA 9.1 Fr 15:15 TU EMH225

Halfmetallic Alloys: Electronic Structure, Magnetism, and Spin Polarisation — •Peter H. Dederichs, Iosif Galanakis, and Phivos Mavropoulos — Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich

Halfmetallic alloys are ferromagnets which show a metallic behaviour for the majority electrons, but a semiconducting behaviour with a band gap at the Fermi level E_F for the minority electrons. The resulting 100% spin polarisation at E_F makes them of strong interest for spin electronics. Based on ab-initio calculations, we review the basic understanding of the electronic structure of half-metallic Heusler alloys. The origin of the gap is the d-d hybridisation between the lower-valent (magnetic) and the higher valent (non- magnetic) transition elements. Due to the band gap, an integer number of minority bands is occupied, so that an ideal Slater Pauling behaviour is obtained: The total moment M per unit cell scales with the total number Z of valence electrons, such that $M = Z - 18$ for the half and $M = Z - 24$ for the full Heusler alloys. We discuss the role of spin orbit coupling which in principle destroys the gap, but in practice is of minor importance, since the spin polarisation remains very high. Also other relativistic effects like orbital moments and magnetic anisotropy energies are typically very small. From application point of view the existence of disorder induced impurity gap states and of surface and interface states in the gap represent the biggest challenge. We shortly discuss the halfmetallic zincblende compounds like CrAs which show many similar properties.

Hauptvortrag MA 9.2 Fr 15:45 TU EMH225

The properties of $Co_2Cr_{1-x}Fe_xAl$ Heusler compounds — •Claudia Felser, Gerhard H. Fecher, Sabine Wurmehl, and Thomas Block — Johannes Gutenberg - Universität, 55099 Mainz, Germany

The compound $Co_2Cr_{0.6}Fe_{0.4}Al$ was prepared, guided by striking features in the electronic structure of several magnetic Heusler compounds. Based on band structure calculations, this composition was chosen in order to obtain a ferromagnetic half metal with a van Hove singularity in the vicinity of the Fermi energy in the majority spin channel and a gap in the minority spin channel. The evidence for spinpolarized transport at room temperature was found, showing up in a magnetoresistive effect of 35% in a small magnetic field of 0.1 Tesla. Heusler compounds with composition $Co_2Cr_{1-x}Fe_xAl$ were prepared by arc melting and comprehensively characterized by means of XRD, SQUID magnetometry, Mößbauer spectroscopy, MXCD, ESCA and AES depth profiling. X-ray diffraction and EXAFS pointed on structural disorder phenomena. Band structure calculations are presented for ordered and disordered compounds. The connection between specific site disorder and the band structure is shown explicitly with particular emphasis on the half-metallic properties. Experimentally observed deviations from the ideal Heusler structure and from the simple Slater-Pauling rule for the magnetization are discussed in close relation to theoretical models.

Hauptvortrag MA 9.3 Fr 16:15 TU EMH225

Elementspecific electronic properties of the Heusler alloys investigated by X-ray absorption spectroscopy — •Hans-Joachim Elmers — Johannes Gutenberg Universität Mainz

Doped Heusler alloys and compounds of the $Co_2(Y_xY'_{(1-x)})Z$ type are potential candidates for halfmetallic ferromagnetic materials that can be used in spintronic devices. The electronic properties can be tuned by varying Mn to Fe and Cr to Fe ratio x on the Y site. Of particular interest are properties at the surface of the material since all potential applications rely on electron transfer through an interface. In order to confirm theoretical investigations, that predict a gap in the minority bands, we performed X-ray absorption spectroscopy at the $L_{3,2}$ edges of the 3d transition metals of the pure compounds (x=0 and x=1) and alloys with varying composition x [1]. The determination of all photoemitted electrons (total yield) provides a moderate surface sensitivity (¡10 nm). For in-situ cleaned bulk samples or in-situ capped surfaces we determine element specific magnetic moments. We compare our measurements with simulated spectra based on ab-initio bandstructure calculations. The absorption spectra show distinct features that can be related to the degree of disorder in the $L2_1$ - Heusler structure. The Cr moment is quenched in disordered areas of the sample because of a partly antiparallel alignment and therefore serves as a tracer signal for fully ordered unit cells. The comparison of XMCD spectra of Cr with simulated spectra indicates a high spinpolarization in ordered compounds.

[1] H. J. Elmers, S. Wurmehl, G. H. Fecher, G. Jakob, C. Felser, G. Schönhense, Appl. Phys. A 79, 2004, 557 and references therein.

Hauptvortrag MA 9.4 Fr 16:45 TU EMH225

Interplay of defects and temperature in NiMnSb — •Robert A. de Groot, Jisk Attema, Liviu Chioncel, Changming Fang, Gilles A. de Wijs, and Alex I. Lichtenstein — ESM, Toernooiveld 1, Nijmegen, The Netherlands

The electronic structure of NiMnSb, the origin of the band gap for one spin-direction as well as the influence of intrinsic defects are discussed. Intrinsic point-defects are unlikely or have a negligible effect but the effect of the surface is detrimental for the half-metallic properties. Genuinely half-metallic interfaces with zinc-blende semiconductors are possible however, and the underlying physics will be discussed. Finally, possibilities of introducting non-intrinsic defects will be explored in order to optimize the spin-polarization of the conduction at finite temperatures through the modification of the magnon density of states.

Hauptvortrag MA 9.5 Fr 17:15 TU EMH225

Magnetism of $[Co_2MnGe/Au]_n$ and $[Co_2MnGe/V]_n$ multilayers — •K. Westerholt, A. Bergmann, J. Grabis, E. Verduijn, A. Nefetov, and H. Zabel — Experimentalphysik/Festkörperphysik Ruhr-Uni-Bochum 44780 Bochum, Germany

The magnetic behavior of the fully spin polarized Heusler compounds at interfaces with dielectrics and non magnetic metals is essential when judging the perspective of these materials as ferromagnetic layers in typical spintronic devices. We review our results on the magnetic and structural properties of multilayers composed of the fully spin polarized Heusler alloy Co_2MnGe with V or Au as interlayers. In $[Co_2MnGe/Au]_n$ multilayers the interlayers cause an exchange bias shift of the ferromagnetic hysteresis loops at low temperatures. The analysis of the x-ray resonant magnetic reflectivity reveals that the magnetization profile of Mn is definitely different from that of Co and asymmetric with respect to the growth direction of the layers. In $[Co_2MnGe/V]_n$ multilayers with very thin Heusler layers we observe an antiferromagnetic interlayer long range ordering below a well defined Néel temperature originating from the dipolar stray fields of the magnetically rather rough Heusler layer interfaces.

Hauptvortrag MA 9.6 Fr 17:45 TU EMH225

Magnetic tunnel junctions with Heusler alloy electrode: Interface structure and magnetism in the shine of soft X-rays — •Jan Schmalhorst — University of Bielefeld, Department of Physics, Nano Device Group, P.O. Box 100131, 33501 Bielefeld, Germany

The implementation of half-metallic materials like full Heusler alloys [1] for spintronic applications [2], e.g., as electrode in magnetic tunnel junctions, is of highest technological relevance. The major challenge is the preparation of preferably defect free interfaces. We fabricate Co_2MnSi / AlO_x / Co-Fe MTJs with 95% tunneling magnetoresistance (TMR) at low temperature and low bias voltage [3,4]. However, the TMR bias voltage and temperature dependence is considerably stronger than usually found for optimized MTJs with 3d-alloy electrodes. For explaining this conclusively, knowledge of the structural and magnetic properties of the Co_2MnSi / AlO_x interface is of vital importance. In this talk investigations of the Co_2MnSi / AlO_x interface [5] and the Co_2MnSi bulk material by X-ray absorption spectroscopy will be presented and discussed with respect to the temperature dependent transport properties of the junctions. The author gratefully acknowledge the opportunity to perform soft X-ray absorption spectroscopy at the Advanced Light Source, Berkeley, USA and at the BESSY mbH, Berlin, Germany.

[1] R. A. de Groot et al., Rev. Lett. 50 (1983) 2024
[2] S.A. Wolf et al., Science 294, 1488 (2001)
[3] S. Kämmerer et al., Appl. Phys. Lett. 85 (2004) 79
[4] J. Schmalhorst et al., to be published

[5] J. Schmalhorst et al., Phys. Rev. B 70 (2004) 024426

Hauptvortrag

MA 9.7 Fr 18:15 TU EMH225

Anomalous electronic and vibrational effects in magnetic shape memory alloys — •Peter Entel[1], Alexey T. Zayak[2], and Waheed A. Adeagbo[1] — [1]Physics Section, University of Duisburg-Essen, Duisburg Campus, 47048 Duisburg, Germany — [2]Department of Physics and Astronomy, Rutgers University, Piscataway, NJ 08854-8019, USA

First-principles calculations are used to address the problem of anomalous electronic and vibrational effects in magnetic Heusler compounds. The ferromagnetic shape memory systems Ni_2Mn(Ga, Ge, Al) undergo a structural transformation from the high-temperature $L2_1$ structure to some low-temperature tetragonal or modulated structure. This can be related to Fermi surface nesting caused by a peculiar combination of electronic states of Ni and, for example, Ga. The resulting tetrahedral-like coordination of the transition metal ions causes also the lattice instability, where the acoustic modes tend to soften while the optical modes disperse in a way which is significantly different from that in stable ferromagnetic Co_2Mn(Ga, Ge). Critical valence electron numbers per atom can still be used to characterize the unstable and stable magnetic alloys. However, in a more detailed descripion the anharmonic behavior of the unstable magnetic systems is related to the Jahn-Teller splitting and an amplification of anharmonicity by competing ferromagnetic and antiferromagnetic interactions. We discuss the close relationship of anharmonic trends observed in ferroelectrics.