MA 22: FV intern Symposium: "Heusler Alloys" Invited Talks Kübler/Yamamoto/Inomata/Silvia Picozzi

Time: Thursday 10:15–13:15 Location: H10

Invited Talk MA 22.1 Thu 10:15 H10

Thermal properties of magnets from *ab initio*. — •Jürgen Kübler — Technische Universität Darmstadt

The local spin-density functional approximation (SDFA) is being successfully used for materials applications such as predicting structural and magnetic properties in the ground state. The ability to model low-lying magnetic excitations in the SDFA by means of non-collinear spin configurations together with well-established techniques from statistical mechanics also allows a determination of thermal properties of itinerant-electron magnets from *ab initio*. The Curie temperature, for instance, can be estimated quite reliably using the spherical approximation. This is demonstrated for a sizable number of Heusler compounds and other magnets for which theoretical predictions constitute an important tool in materials development. *I gratefully acknowledge helpful discussions with Claudia Felser and Gerhard Fecher (Universität Mainz). I am, furthermore, indebted to Claudia Felser and Burkhard Hillebrands for their support.*

Invited Talk MA 22.2 Thu 10:45 H10

Highly spin-polarized tunneling in fully epitaxial magnetic tunnel junctions with a Co-based full-Heusler alloy thin film and a MgO barrier — •Masafumi Yamamoto, Takao Marukame, Takayuki Ishikawa, Ken-ichi Matsuda, and Tetsuya Uemura — Division of Electronics for Informatics, Hokkaido University, Sapporo 060-0814, Japan

Co-based full-Heusler alloy (Co_2YZ) thin films are highly preferable ferromagnetic materials in spintronic devices. This is because of the half-metallic ferromagnetic nature theoretically predicted for some of these alloys, and because of their high Curie temperatures, which are well above room temperature (RT). We developed fully epitaxial magnetic tunnel junctions (MTJs) with a Co_2YZ thin film and a MgO tunnel barrier (Refs. 1-3), and showed a relatively high tunnel magnetoresistance ratio of 109% at RT (317% at 4.2 K) for $Co_2Cr_{0.6}Fe_{0.4}Al$/MgO/$Co_{50}Fe_{50}$ MTJs (Ref. 3). Furthermore, the bias voltage dependence of differential conductance of Co_2MnSi/MgO/$Co_{50}Fe_{50}$ MTJs for the parallel and antiparallel magnetization configurations suggested the existence of a basic energy gap structure for the minority-spin band of the Co_2MnSi electrode (Ref. 2). These results confirm the promise of epitaxial MTJs as a key device structure for utilizing the potentially high spin polarization of Co_2YZ thin films. 1) T. Marukame *et al.*, *Appl. Phys. Lett.* 88, 262503 (2006). 2) T. Ishikawa *et al.*, *Appl. Phys. Lett.* 89, 192505 (2006). 3) T. Marukame *et al.*, to be published in *Appl. Phys. Lett.*

Invited Talk MA 22.3 Thu 11:15 H10

giant tunnel magnetoresistance at room temperature using Co2Fe(SiAl) full Heusler alloy electrodes — •koichiro inomata[1,2,3], naomichi ikeda[2], and nobuki tezuka[2,3] — [1]National Institute for Materials Science, Tsukuba, Japan — [2]Tohoku University, Sendai , Japan — [3]CREST-JST, Saitama, Japan

Half-metallic ferromagnets (HMFs) are a key material for spintronics, which have a band gap at the Fermi level (EF) for one spin direction and thus exhibit 100% spin polarization at the EF. Full Heusler alloys, in particular, are promising as a half metal, because a number of which have been predicted to be HMFs and have a high Curie temperature. Here we report the giant TMR observation at room temperature (RT) for the MTJ using Co2Fe (Si,Al) (CFSA) electrodes. We first investigate the structure of the sputtered CFSA films on a Cr-buffered MgO (001) substrate in an ultrahigh vacuum by post annealing at various temperatures. Next we fabricate the epitaxially grown spin-valve type MTJs on a Cr-buffered MgO (001) substrate with Co2FeSi0.5Al0.5 full-Heusler alloys for top and bottom electrodes and an MgO barrier with different thicknesses. The bottom CFAS film is post-annealed at 673 K after the deposition at RT, followed by the deposition of the other films at RT. The junctions are the annealed at various temperatures, and then microfabricated into 100 mm2 using the electron beam lithography and Ar ion milling. We have successfully grown the highly ordered CFSA full-Heusler films for top and bottom electrodes. As a result we have attained the giant TMR over 200% at RT.

Invited Talk MA 22.4 Thu 11:45 H10

First-principles study of ferromagnetic Heusler alloys: an overview — •Silvia Picozzi — CNR-INFM CASTI Regional Lab, 67010 L'Aquila (Italy)

On the basis of ab-initio results, I will review several aspects of ferromagnetic Co2MnX (X = Si, Ge and Sn) Heusler alloys, predicted to be half-metallic and, as such, promising candidates for spin-injection purposes. In particular, I will focus on:

i) Bulk magneto-optical properties: after a brief review of their electronic and magnetic properties, a careful analysis of magneto-optical spectra, in comparison with experiments, will be presented.

ii) Polarization reduction mechanisms. Our results show that in Heusler compounds a) intrinsic point-defects can be detrimental for half-metallicity and b) when joined to mainstream semiconductors, the presence of interface states at the Fermi level can degrade their performances. In particular, I will focus on Co2MnSi and Co2MnGe, in the presence of intrinsic defects (such as stoichiometric atomic swaps as well as non-stoichiometric antisites) and interfaced with GaAs and Ge. Antisites, due to their low formation energies, can easily occur, consistently with experiments; however, only Co antisites give rise to defect-states at the Fermi level. As for the [001]-ordered interfaces, the strong hybridization at the junction gives rise to broad interface states which locally destroy half-metallicity. Finally, in the context of multiferroic tunnel junctions, preliminary results for Heuslers interfaced with ferroelectrics will also be presented.

MA 22.5 Thu 12:15 H10

Huge magneto-optical Kerr effect and its modification by ion irradiation in the Co_2FeSi Heusler compound — •J. Hamrle[1], O. Gaier[1], S. Blomeier[1], H. Schneider[2], G. Jakob[2], B. Reuscher[3], A. Brodyanski[3], M. Kopnarski[3], C. Felser[4], and B. Hillebrands[1] — [1]FB Physik and Forschungsschwerpunkt MINAS, TU Kaiserslautern, E.-Schrödinger-Str. 56, D-67663 Kaiserslautern — [2]Institut für Physik, J.-Gutenberg-Universität, Staudinger Weg 7, D-55128 Mainz — [3]IFOS TU Kaiserslautern, E. Schrödinger-Str. 56, D-67663 Kaiserslautern — [4]Institute of Chemistry, J.-Gutenberg-Universität, Staudingerweg 9, D-55128 Mainz

Heusler alloys are promising candidates for spintronics devices providing 100% spin polarization. We report on magnetic and magneto-optical properties of thin Co_2FeSi (CFS) Heusler films measured by means of magneto-optical Kerr effect (MOKE). CFS films sputtered on MgO(100) grow in the fully ordered $L2_1$ structure. MOKE hysteresis loops measured on CFS films exhibit a large quadratic (QMOKE) and longitudinal MOKE (LMOKE) contribution, resulting in asymmetrical MOKE loops. The amplitude of the QMOKE is 30 mdeg, the largest QMOKE found so far. It is a hint of an unusually large second-order spin-orbit (SO) coupling in CFS films. We studied the effect of structural disorder on the magnetic properties by irradiating the CFS samples with different fluences of 30 keV Ga^+ ions. Results shows that small doses reduce the second-order SO coupling while keeping unmodified the first order SO coupling. Supported by the DFG in the FG 559 and by the Japanese government in the NEDO 2004IT093.

MA 22.6 Thu 12:30 H10

Structural characterization of Heusler compounds using NMR — •Sabine Wurmehl[1], Marek Wojcik[2], Gerhard Fecher[1], Benjamin Balke[1], Vadim Ksenofontov[1], Verena Jung[1], and Claudia Felser[1] — [1]Johannes Gutenberg - Universität, 55099 Mainz, Germany — [2]Institute of Physics, Polish Academy of Sciences, 02-668 Warszawa, Poland

The $L2_1$ ordered Heusler alloys $Co_2Mn_{1-x}Fe_xSi$ with $0 \leq x \leq 1$ attracted much scientific interest, as they are predicted to show high spin polarisation at the Fermi-energy.

Therefore $Co_2Mn_{1-x}Fe_xSi$ samples were investigated using spin echo nuclear magnetic resonance (NMR) measurements. This method provides a tool to measure the hyperfine fields. The hyperfine fields represent a very sensitive local probe to order-disorder phenomena.

The NMR measurements of polycrystalline Co_2FeSi samples exhibit a two-peak spectrum with an additional shoulder. This additional signals are attributed to second-order quadrupole splitting, a so called

asymmetric line broadening and might be caused by tension within the structure (strain). This effect occurs even in highly ordered systems. Thus previous structural results are corroborated, demonstrating even locally a very high degree of order in Co_2FeSi.

The NMR spectra of the series $Co_2Mn_{1-x}Fe_xSi$ ($(0.1 \leq x \leq 0.9)$) exhibit multiplet structures. These might be explained by quadrupole splitting and statistical distribution of Mn and Fe atoms on the Mn site. In summary, the high degree of order in $Co_2Mn_{1-x}Fe_xSi$ is shown.

(This work is funded by the DFG in FG 559.)

MA 22.7 Thu 12:45 H10

Heusler compounds implemented in magnetic tunnel junctions: basic properties and applications — •Jan Schmalhorst, Andy Thomas, Andreas Hütten, and Günter Reiss — Bielefeld University, Department of Physics, Thin Films and Nanostructures, P.O. Box 100131, 33501 Bielefeld, Germany

The implementation of half-metallic materials like Heusler compounds [1] in magnetic tunnel junctions for spintronic applications is of highest technological relevance [2]. The major challenge is the preparation of defect free thin Heusler compound films and high quality electrode - barrier interfaces. In this talk, we will compare transport as well as magnetic and chemical bulk and interface properties of tunnel junctions with Co2MnSi, Co2FeSi, Co2FeMnSi or CoMnSb electrodes and Al-O or Mg-O barrier. Especially, we will focus on the bias voltage dependent inversion of the tunnel magnetoresistance [3, 4], which can be utilized for programmable logic devices [5]. The author gratefully acknowledge financial support by DFG and EU and the opportunity to perform soft X-ray absorption spectroscopy at the Advanced Light Source, Berkeley, USA.

[1] R. A. de Groot et al., Phys. Rev. Lett. 50 (1983) 2024
[2] S.A. Wolf et al., Science 294 (2001) 1488
[3] D. Ebke, J. Schmalhorst et al., Appl. Phys. Lett. 89 (2006) 16250
[4] J. Schmalhorst et al., Phys. Rev. B, accepted
[5] A. Thomas et al., Appl. Phys. Lett. 89 (2006) 012502

MA 22.8 Thu 13:00 H10

Electronic structure and high energy valenceband photoemission of Heusler compounds — •Gerhard H. Fecher and Claudia Felser — Institute for Inorganic and Analytical Chemistry, Johannes Gutenberg - Universität, 55099 Mainz, Germany

This work reports on high resolution photoelectron spectroscopy of the valence band of $Co_2Mn_{1-x}Fe_xSi$ ($x = 0, 0.5, 1$) excited by photons of 8 keV energy. The measurements show a good agreement to calculations of the electronic structure using the LDA+U scheme. It is shown that the high energy spectra reveal the bulk electronic structure better compared to low energy XPS spectra. The high resolution measurements of the valence band close to the Fermi energy indicate the existence of the gap - or at least a pronounced minimum - in the minority states for all three alloys.

The role of the composition for the position of the Fermi energy and the stability of the half-metallic ferromagnetism is discussed for the iso-electronic Heusler compound $Co_2FeAl_{1-x}Si_x$. The energy dependence of high energy photoelectron spectroscopy will be discussed with an example of spectra taken at 1.2-5 keV from the $C1_b$ compound CoTiSb.

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