MA 4: Spin-dependent Transport Phenomena

Time: Monday 9:30–13:00 Location: H 1012

MA 4.1 Mon 9:30 H 1012

Extrinsic spin Hall effect in metallic films from first principles — •Christian Herschbach[1,2], Martin Gradhand[3], Dmitry Fedorov[1,2], Peter Zahn[2], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Hall, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [3]H. H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1TH, United Kingdom

We present ab initio calculations of the skew scattering contribution to the spin Hall effect for free-standing fcc Au(111) films with substitutional Pt impurities. Their thickness is varied between 1 and 32 monolayers. The calculated spin Hall angle changes drastically as a function of impurity position within the film. We show that adatoms play a special role. In particular, they cause a sign change of the spin Hall angle. Moreover, Pt adatoms on a 1 monolayer Au film give rise to a drastic enhancement of the spin Hall angle.

MA 4.2 Mon 9:45 H 1012

Investigation of the extrinsic spin Hall effect in transition metal alloys — •K Chadova, D Ködderitzsch, and H Ebert — Universität München, Department Chemie, Butenandtstr. 5-13, D-81377 München

The extrinsic spin Hall effect (SHE) can be controlled by manipulating the concentration of impurities or by changing the impurity and host materials. In the present work we investigate the extrinsic SHE in transition metal alloys in the dilute limit from first principles. The calculations were performed by using the fully relativistic Korringa-Kohn-Rostoker (KKR) Green's function method in combination with the Coherent Potential Approximation (CPA) alloy theory on the basis of the Kubo-Streda equation.

A large extrinsic SHE is observed when the spin-orbit coupling (SOC) strength of the impurity is substantially different from the host. The magnitude of the calculated extrinsic SHE is found to scale approximately with the ratio of SOC of impurity and the host materials. In particular, we observe a sign change in the extrinsic spin Hall conductivity for some impurities. The latter depends on the relation between SOC strengths of the host and the impurtity. These results are found in a reasonable agreement with available experimental data.

MA 4.3 Mon 10:00 H 1012

The Planar Hall Effect in exchange-biased nanocrystalline $Co_{60}Fe_{20}B_{20}$ — •Klaus Seemann[1], Frank Freimuth[2], Florian Kronast[3], Sergio Valencia[3], Hongbin Zhang[2], Stefan Blügel[2], Yuriy Mokrousov[2], Daniel Bürgler[1], and Claus Schneider[1] — [1]Peter Grünberg Institut (PGI-6) and Jülich-Aachen Research Alliance (JARA-FIT), Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Peter Grünberg Institut (PGI-1), Institute for Advanced Simulation, and Jülich-Aachen Research Alliance (JARA-FIT), Forschungszentrum Jülich, D-52425 Jülich, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

An angle dependent analysis of the planar Hall effect (PHE) in nanocrystalline single-domain $Co_{60}Fe_{20}B_{20}$ thin films is reported. In a combined experimental and theoretical study we show that the transverse resistivity of the PHE is entirely driven by anisotropic magnetoresistance (AMR). Our results for $Co_{60}Fe_{20}B_{20}$ obtained from first principles theory in conjunction with a Boltzmann transport model take into account the nanocrystallinity and the presence of 20 at. % boron. The ab initio AMR ratio of 0.12% agrees well with the experimental value of 0.22%. We demonstrate that the anomalous Hall effect contributes negligibly in the present case. We complete our study by field dependent and element specific microscopic investigations based on X-ray magnetic dichroism (XMCD-PEEM) of exchange biased $Co_{60}Fe_{20}B_{20}$.

[1] K. M. Seemann et al., Phys. Rev. Lett. 107, 086603, 2011

MA 4.4 Mon 10:15 H 1012

Side-Jump Scattering Contribution to Anomalous Hall Effect from Magnetic Impurities — •Jürgen Weischenberg, Frank Freimuth, Stefan Blügel, and Yuriy Mokrousov — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Recently, within the full-potential linearized augmented plane-wave scheme (FLAPW), we have implemented a method that allows for a calculation of the intrinsic [1] and side-jump (SJC) scattering-independent contributions to the anomalous Hall effect (AHE) from the electronic structure of a perfect crystal alone [2], assuming that the disorder in the system is short-ranged. Although the SJC depends neither on the impurity concentration nor the scattering strength, it is sensitive to the spin structure of the impurity potential, which makes it possible to consider different scenarios for side-jump scattering from magnetic impurities. We extended and applied our method to study the effects of scattering from magnetic impurities on the AHE in a variety of ferromagnetic materials. We also analyze the role of spin-flip processes for the AHE, which have been considered previously for the intrinsic contribution. Financial support by the HGF-YIG Programme VH-NG-513 is gratefully acknowledged.

[1] H. Zhang, F. Freimuth, S. Blügel, Y. Mokrousov and I. Souza, PRL **106**, 117202 (2011)

[2] J. Weischenberg, F. Freimuth, J. Sinova, S. Blügel and Y. Mokrousov, PRL **107**, 106601 (2011)

MA 4.5 Mon 10:30 H 1012

Tunnel-induced spin-anisotropy in quantum dot spin valves — •Maciej Misiorny[1], Michael Hell[1], and Maarten Wegewijs[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich & JARA Jülich Aachen Research Alliance, 52425 Jülich, Germany — [2]Institute for Theory of Statistical Physics, RWTH Aachen, 52056 Aachen, Germany

Atomic-scale spintronic systems, such as single-molecule magnets (SMMs) and magnetic adatoms, have recently been studied intensely mainly because of their large spin-anisotropy arising from strong spin-orbit and ligand fields. We show that spin-anisotropy can also be generated in *spin-isotropic* systems by spin-dependent transport of electrons. For a generic spin-1 quantum dot tunnel coupled to two metallic ferromagnetic electrodes we show that quantum fluctuations induce a *quadrupolar exchange field*, generalizing the well established (dipolar) exchange field. This field generates a uniaxial spin-anisotropy barrier that increases with the tunnel coupling, achieving values comparable to that of SMMs, but with the added flexibility of electric and magnetic tuneability. Besides inducing it, the transport can also be used to directly read out the quadrupolar field, utilizing its competition with Kondo spin-exchange processes with the ferromagnets. In this regime the proximity-induced quadrupolar exchange field is found to dominate over the dipolar exchange field, strongly enhancing the low-temperature spin-filtering as compared to spin-1/2 quantum dot spin-valves. Consequently, not only do spin-quadrupole effects in spin-polarized transport seem inevitable in high-spin nanosystems, but they also offer new prospects for spintronic applications.

MA 4.6 Mon 10:45 H 1012

Spin polarized tunneling in MgO-based tunnel junctions with superconducting electrodes — •Oliver Schebaum[1], Günter Reiss[1], Jagadeesh S. Moodera[2], and Andy Thomas[1] — [1]Thin Films and Physics of Nanostructures, Physics Department, Bielefeld University, Germany — [2]Francis Bitter Magnet Laboratory, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

We prepared magnetic tunnel junctions with one ferromagnetic and one superconducting Al-Si electrode. Pure cobalt electrodes were compared with a Co-Fe-B alloy and the Heusler compound Co_2FeAl. The polarization of the tunneling electrons was determined using the Maki-Fulde-model and is discussed along with the spin-orbit scattering and the total pair-breaking parameters. The junctions were post-annealed at different temperatures to investigate the symmetry filtering mechanism responsible for the giant tunneling magnetoresistance ratios in Co-Fe-B/MgO/Co-Fe-B junctions.

MA 4.7 Mon 11:00 H 1012

Ultrafast Transport of Laser-Excited Spin-Polarized Carriers in Metallic Multilayers — •Alexey Melnikov[1], Alexandr Alekhin[1], Tim O. Wehling[2], Vladimir V. Roddatis[3], Damian Bürstel[4], Detlef Diesing[4], Alexander I. Lichtenstein[2], and Uwe Bovensiepen[5] — [1]Fritz-Haber-Institut der MPG, Abt. Phys. Chemie — [2]Universität Hamburg, Theor. Phys. Institut — [3]CIC Energigune, Spain — [4]Universität Duisburg-Essen, Institut für Phys.

Chemie — [5]Universität Duisburg-Essen, Fakultät für Physik

The ultrafast spin dynamics (SD) induced by a transport of spin polarized carriers is a hot topic motivated by the fundamental interest in magnetic excitations and applications like spintronics and data storage. To understand underlying elementary processes typically occurring on femtosecond time scales, we have developed a time-of-flight-like approach that probes SD induced by hot carriers (HC) and demonstrated a spin polarized HC transport through an epitaxial Au/Fe/MgO(001) structure. Using a back pump-front probe configuration, we establish that HC induced in Fe by the pump laser pulse can form a nearly ballistic spin current in Au: optical second harmonic (SH) generated at the Au surface by the probe pulse monitors the transient surface HC density and spin polarization formed by predominantly ballistic/diffusive spin-down/up carriers. Comparing the SH response of Fe to the direct optical excitation with that to the excitation by hot carriers generated in Au, we rule out coherent effects of the pump pulse and show that the HC-induced SD is the main origin of the ultrafast demagnetization. Financial support by the DFG through ME 3570/1-1 is acknowledged.

15 min. break

MA 4.8 Mon 11:30 H 1012

Static and dynamic properties of magnetic domain configurations in patterned La0.7Sr0.3MnO3 nanostructures — •Luís Peña[1], Carlos Vaz[1,2], Michael Förster[1], Jan Rhensius[2,3,4], Andrè Bisig[2,4,8], Phillip Wolhüter[2,4], Sebastian Schweitzer[4], Jakoba Heidler[2], Helmut Körner[2,4], Andrea Locatelli[5], Miguel Niño[5], Markus Weigand[6], Laurence Méchin[7], Fabien Gaucher[7], Eberhard Goering[8], Souliman Moussaoui[9], Frithjof Nolting[9], Laura Heyderman[3], and Mathias Kläui[1] — [1]Institut für Physik, JGU Mainz, Staudingerweg 7, D-55128 — [2]SwissFEL, PSI, CH-5232 — [3]Lab. for Micro- and Nanotech., PSI, CH-5232 — [4]Fachbereich Physik, Univ. Konstanz, Universitätsstraβe 10, D-78457 — [5]Sincrotrone Trieste, I-34149 — [6]HZB für Mater. und Energ. GmbH,D-12489 — [7]GREYC, 6 Blvd. du Maréchal Juin,FR-14050 — [8]Max-Plancx-Instute for Intelligent System, Heisenbergstrasse 3, D-70569 — [9]SLS-PSI, CH-5232

The static magnetic domain configuration in square- and ring-shape structures is investigated by direct high-resolution x-ray magnetic microscopy as a function of temperature and geometrical parameters. We show that the magnetic configurations evolve from multidomain to flux-closure states with decreasing element size, with a thickness-dependent crossover at the micrometric scale. The flux-closure states are stable against thermal excitations up to near the Curie temperature. Through magnetotransport experiments on half-ring structures we investigate the dynamic properties of transversal domain wall depinning by current pulse injection.

MA 4.9 Mon 11:45 H 1012

Magnetotransport properties of Pd-rich PdFe alloys: effect of chemical ordering — •Josef Kudrnovsky[1], Ilja Turek[2], Vaclav Drchal[1], and Sergei Khmelevskii[3] — [1]Institute of Physics AS CR, Prague — [2]Institute of Physics of Materials AS CR, Brno — [3]CMS, University of Technology, Vienna

The electronic structure and transport properties of Pd-rich PdFe alloys are investigated as a function of the atomic and magnetic orders. The densities of states, magnetic moments, residual resistivites, anisotropic magnetoresistances (AMR), and the anomalous Hall effect (AHE) are calculated from first-principles. The atomic order is characterized by an amount of antisite Pd-Fe disorder on Pd- and Fe-sublattices. Both stoichiometric Pd3Fe and non-stoichiometric Pd(70)Fe(30) alloys are studied. The electronic structure is determined in the framework of the TB-LMTO method in which the effect of disorder is described by the coherent potential approximation (CPA). The conductivity tensor from which the AMR and AHE are calculated, is determined from relativistic generalization of the transport Kubo-Greenwood approach. The effect of the thermal magnetic disorder on the resistivity and the AMR has been studied in the framework of the disordered local moment approach based on CPA. Our results are in an overall good agreement with available experimental data.

MA 4.10 Mon 12:00 H 1012

$Mn_{3-x}Ga$ based magnetic tunnel junctions with perpendicular magnetic anisotropy — •Manuel Glas, Daniel Ebke, Markus Schäfers, Patrick Thomas, and Günter Reiss — Thin Films and Physics of Nanostructures, Bielefeld University, Germany

The integration of $Mn_{3-x}Ga$ thin films with perpendicular magnetic anisotropy into magnetic tunnel junctions was investigated. MgO (001) and $SrTiO_3$ (001) substrates were used to achieve epitaxial (001)-oriented thin films. Crystallographic and magnetic measurements were performed to characterize the $Mn_{3-x}Ga$ electrodes. A strong Mn oxidation at the barrier interface was found from X-ray absorption spectroscopy (XAS). Therefore, a thin protection layer of CoFeB or Mg was deposited to improve the quality of the interface between barrier and electrode. A magnetically perpendicular counter electrode was formed by Co/Pt multilayers. Major loop hysteresis measurements suggest a magnetic decoupling between the electrodes through the MgO barrier. First transport measurements showed a maximum room temperature TMR ratio of 18 % for $Mn_{2.3}Ga$/CoFeB/MgO/CoFeB/$\{Co/Pt\}_{10}$ on MgO and 14 % on $SrTiO_3$ substrates. The corresponding low temperature (13 K) TMR values reach 32 % for MgO and 26 % for $SrTiO_3$ substrates. The obtained transport properties will be compared to Co/Pd based magnetic tunnel junctions with perpendicular magnetic anisotropy.

MA 4.11 Mon 12:15 H 1012

Calculation of Fermi surfaces and Elliott-Yafet parameter from first principles — •B. Zimmermann, S. Heers, N. H. Long, Y. Mokrousov, P. Mavropoulos, and S. Blügel — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The knowledge of the Fermi surface (FS) is crucial for the understanding of many properties of metals. For example, spin-dependent electron transport phenomena are determined by the electronic structure of a material in the vicinity of its FS. In the first-principles Korringa-Kohn-Rostoker (KKR) Green-function method [1], the band structure is determined by the zeros of the determinant of the non-hermitian KKR matrix, $\det(\mathcal{M}(\mathbf{k}, E)) = 0$. Many $\mathbf{k}$-points are required to obtain an accurate description. Here, we report on the implementation of a tetrahedron method within the KKR framework in which the spin-orbit interaction has been included. Our approach is based on an interpolation of the complex eigenvalues of $\mathcal{M}$ at a fixed energy $E = E_F$ instead of an interpolation of $E(\mathbf{k})$. This allows for a fast and accurate calculation of complex FSs of slab and bulk systems. As an application of the method, we investigate the Fermi-surface topology and the Elliott-Yafet spin-mixing parameter of 5*d* transition metals.

We acknowledge funding under DFG project MO 1731/3-1 and HGF-YIG program VH-NG-513.

[1] N. Papanikolaou, R. Zeller, P. H. Dederichs, J. Phys.: Condens. Matter **14**, 2799 (2002).

MA 4.12 Mon 12:30 H 1012

Interlayer exchange coupling and transport properties of SrTiO3 based magnetic tunnel junctions — •Brahim Belhadji[1], Hongxin Yang[1], Julian Velev[2], and Mairbek Chshiev[1] — [1]Spintec, UMR, CEA/CNRS/UJF Grenoble, France — [2]University of Puerto Rico, San Juan, Puerto Rico 00931, USA

In view of further miniaturization of spintronic devices, alternative to MgO materials are required in order to maintain a high TMR as resistance-area product becomes smaller. A possible solution may be SrTiO3 due to its smaller bandgap compared to MgO. Here we present first-principle calculations of interlayer exchange coupling(IEC) and spin dependent transport in SrTiO3-based MTJs as a function of barrier thickness and electrode composition (Fe, FeCo and Co). We found that the IEC is antiferromagnetic for relaxed Co/SrTiO3/Co structures and decays exponentially as a function of SrTiO3 thickness and stronger compared to Fe|MgO|Fe. Furthermore, in case of CoFe|SrTiO3 MTJs the IEC amplitude has a clear tendency to decrease and even become positive as Fe content increases. Spin dependent transport calculations in these MTJs show that SrTiO3 seems not to be as good a spin filter as the MgO even though TMR values of 3000% for 9 monolayers of SrTiO3 (~ 1.6nm) were obtained for Co|SrTiO3|Co MTJs, in agreement with previous studies. We also calculated the dependence of TMR on the electrode composition and barrier oxidation conditions.

This work has been supported by French National Research Agency (ANR) Project CRYSTO and by Nanosciences Foundation in Grenoble, France.

MA 4.13 Mon 12:45 H 1012

***Ab initio* investigation of the Elliott-Yafet parameter in symmetric ultrathin W films** — •N. H. Long, P. Mavropoulos, S. Heers, B. Zimmermann, Y. Mokrousov, and S. Blügel

— Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The spin relaxation in non-magnetic metallic thin films is an important effect in spintronics [1]. In systems with space-inversion symmetry, the spin relaxation is mainly due to the Elliott-Yafet mechanism [2,3]: momentum scattering ($|\mathbf{k}\rangle \rightarrow |\mathbf{k}'\rangle$) at impurities or phonons can cause spin-flip scattering due to the presence of spin-orbit coupling of degenerate Bloch states, that entails a $\mathbf{k}$-dependent superposition of spin-up and -down states. Within this model, momentum- and spin-relaxation rate are proportional. The proportionality factor is the Elliott-Yafet parameter b^2, which quantifies the degree of admixture of states with different spin character in a crystal. In this work, we calculate the b^2 parameter of symmetric W(100) and W(110) ultrathin films using the Korringa-Kohn-Rostoker Green function method. Our results reveal an oscillation of the b^2 parameter as a function of thickness of the films, as well as a significant anisotropy. We discuss our findings in terms of the symmetry properties of bulk and surface states on the Fermi surface of the films. We acknowledge funding from DFG under MO 1731/3-1 and HGF-YIG Programme VH-NG-513.

[1] I. Žutić, J. Fabian, S. Das Sarma, Rev. Mod. Phys. **76**, 323 (2004).

[2] R. J. Elliott, Phys. Rev. **96**, 266 (1954).

[3] Y. Yafet, Solid State Physics, Vol. **14**, 2 (1963).