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“New materials for spintronics, theory and experiment”

Abstracts Talks

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Electron correlations in solids and application to Heusler compounds

S. Chadov

Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55099 Mainz, Germany

chadov@uni-mainz.de

The unusual features of the electronic structure of Heusler alloys which are not captured by widely used Density Functional Theory are studied by taking into account local Coulomb correlations. The latter are described by the Dynamical Mean Field theory (DMFT) combined with ab-initio electronic structure methods, such as KKR (Korringa-Kohn-Rostoker) Green's Function and LMTO (Linearized Muffin-Tin Orbitals). The use of the perturbational impurity solver for the DMFT makes possible to incorporate the account of correlations in a fully self-consistent way (i.e. parallel with the charge self-consistency).
Thus the solution of the many-electron problem is achieved with the high precision.

Our analysis concerns first of all the influence of the dynamical and the static correlations on their integral (magnetic moments) and spectral (magneto-optics, x-ray photoemission) properties.

In addition, we consider the formation of the so-called non-quasiparticle (NQP) states which arise in the minority (majority) spin gap above (below) the Fermi level and which may have a considerable contribution to the electronic properties of half-metallic ferromagnets.

Time-resolved photoemission (and application to Heusler compounds)

M. Chinchetti

Fachbereich Physik, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany

cinchett@rhrk.uni-kl.de

In this lecture I will introduce the concept of time-resolved photoemission and give a brief overview on the application of time-resolved photoemission techniques for the real-time study of surface electronic properties.
Particular emphasis will be given to time-resolved experiments accessing the electron dynamics in ferromagnetic materials, including Heusler alloys. In particular, I will discuss in detail the time-resolved two-photon photoemission. In this context I will describe the main mechanisms influencing the lifetime of excited electrons (or “hot

electrons") in metals. I will show that in ferromagnetic materials the hot-electron lifetime is spin-dependent, resulting in the so-called "spin filter effect" which is the key for understanding the spin properties of spintronics devices.

Halfmetals are not semimetals:

A primer to magnetic states of metals and matter

G.H. Fecher

Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55099 Mainz, Germany

fecher@uni-mainz.de

A short introduction on magnetic and electromagnetic phenomena will be given. Starting point will be the "*Maxwell's equations*" to introduce the basic set of physical quantities and their units being needed to describe the magnetic materials. This is followed by a short brush up of the basic magnetic phenomena in atoms (dia- and para-magnetism) and solids where one has in addition the collective, spontaneous ordering (ferro-, antiferro-, ferri-magnetism, as well as some special cases).
Very often, physical phenomena have nearly the same name but a completely different meaning. A try will be made to resolve some of the related expressions. For example, **semimetals** exhibit the well known phenomenon that the electric conductivity depends on the direction of the electric field *E* with respect to the crystallographic directions. A typical example is graphite being a semiconductor if *E* is along the c-axis and a metal for a current in the plane of the honeycomb lattice. On the other side, a **halfmetal** is a ferromagnet with peculiar transport properties. It shows a semiconductor like behavior in one spin direction and a metallic like conductivity for the other. That means, the conductivity will depend on the direction of *E* with respect to the magnetization. Another example is given by the completely compensated ferrimagnets that behave like antiferromagnets because they do not carry a net magnetic moment. They are different, however, as is easily seen if considering the correct symmetry. Finally, some answers will be given on the questions: "Why is Fe a *weak* ferromagnet and Ni a strong one", "Why is *weak* ferromagnetism observed in Dy", and "Why are ferromagnetic materials close to the Curie temperature *weak*ly ferromagnetic".

Half-metallic epitaxial Fe_3O_4 and CrO_2 Films: spin polarization and magnetotransport

M. Fonin

Universität Konstanz; FB Physik/LS Rüdiger; Universitätstr. 10; 78457 Konstanz

Mikhail.Fonin@uni-konstanz.de

Potential applications of systems based on half-metallic ferromagnets (HMFs) in magneto- and spinelectronics including spin injectors, magnetic field sensors and magnetic memory devices stimulated the investigation of the electronic properties of HFMs by a multitude of experimental and theoretical approaches. The main question remains however if the 100% spin polarization at the Fermi level theoretically predicted for HFMs can be confirmed experimentally. In this talk two half-metallic ferromagnets, namely magnetite (Fe3O4) and chromium dioxide (CrO2), will be discussed with the main emphasis on the spin-resolved photoemission spectroscopy (SP-PES) investigations performed on these materials. Additionally, the results on the investigation of the magnetic domain configurations and the magnetization reversal as well as current injection in magnetic microstructuers fabricated from either Fe3O4 or CrO2 will be presented.

High energy photoemission and application to Heusler compounds

A. Gloskovskii

Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55099 Mainz, Germany

gloskovs@uni-mainz.de

Photoemission is widely used tool for investigation of electronic properties of solids. In Hard X-ray Photoemission Spectroscopy
(HAXPES) the electrons are excited by photons with energies more than 3keV probing bulk properties in contrast to surface sensitive studies under soft X-ray excitation. We will discuss in detail the depth distribution of the photoemitted electrons depending on the excitation energy and experiment geometry. The results of the HAXPES studies of Heusler bulk samples and thin films will be presented.

Imaging, synthesis and fabrication with Synchrotron X-rays

Y. Hwu (胡宇光)

Institute of Physics, Academia Sinica, Taipei, Taiwan

phhwu@gate.sinica.edu.tw

Assisted by the high coherence of synchrotron X-rays, new strategies emerged and start impact research in area of microscopy, fabrication and nanomedicine. In X-ray microscopy, radiography has reached a new level of sophistication and power. Phase contrast due to the difference in the refractive index is added to the absorption as a much improved contrast mechanism. Together with the improvement in the detecting system, we can now looking deep inside into matters with unprecedented precision and speed. Sub-µm or better resolution radiograph can now be obtained with ease and in many cases fast phenomenon can be observed with time resolution better than tens of microsecond. The application of this new tool has already helped researches in materials science, biology and medicine. Ongoing developments in the instrumentation and reconstruction algorithms have generated even higher excitement with the recent demonstration of 30nm scale resolution in 3D with nanofabricated x-ray optical devices. It is anticipated that with the new installation of new low emittance synchrotron source and X-ray free electron laser, X-rays will be able to "image" nanoscale particles and single protein molecule with atomic resolution in the near future and to continue the legacy started by Röntgen.

The intense x-rays are also used to fabricate nanostructures, mostly by x-ray lithography and LIGA techniques. Combined with state-of-the-art electron beam lithography and nanoelectrodeposition, the successful fabrication of X-ray zone plate with 30nm outermost zones and an aspect ratio >15 has reciprocated the development of X-ray microscopy.

The very same X-ray photons are used to synthesize nanoparticles of metals, oxides and polymers with great efficiency and control. These previously unknown capabilities of X-rays now open the door to a number of new therapeutical methods which relies on x-ray targeted drug release, enhanced x-ray radiotherapy and microbeam therapy. Very positive results from NSRRC on the area of early disease detection and nanomedicine provide strong evidence that these new therapeutical strategies might be relevant to human health in the near future.

Thin film deposition methods

M. Jourdan

Institute of Physics, Johannes Gutenberg - University, 55099 Mainz, Germany

jourdan@uni-mainz.de

This presentation will give an overview of deposition methods for epitaxial thin films. The focus will be on Molecular Beam Epitaxy (MBE) and Sputter Depositon. Chemical Vapour Deposition (CVD) and Pulsed Laser Deposition (PLD) are covered briefly. Finally examples of epitaxial growth of intemetallic compounds are discussed.

Multiferroics and Magnetoelectrics: New spintronic routes

Wolfgang Kleemann

Angewandte Physik, Universität Duisburg-Essen, 47048 Duisburg Essen, Germany

wolfgang.kleemann@uni-due.de

Magnetoelectric (ME) materials with a bilinear magnetic and electric free energy contribution, $\Delta F_{me} = -\alpha H \cdot E$, have become of utmost interest, in view of both fundamental understanding and novel desirable applications (Fiebig, 2005). Multiferroic materials with simultaneous polar and magnetic long-range order are expected to optimize the crosslinked responses, *viz.* magnetization excited by electric fields and polarization induced by magnetic ones (Eerenstein *et al.*, 2005). An extension of the conventional multiferroics scenario towards a ME multiglass is found for (Sr,Mn)TiO_3. It shows both dipolar-glass and spin-glass freezing and higher order ME coupling (Shvartsman *et al.,* 2008). Most promising applications in spintronics are presently proposed for the ME multiferroic $BiFeO_3$ (Béa *et al.*, 2008; Ramesh *et al.*, 2008), for the non-ME multiferroic $BiMnO_3$ (Gajek *et al.*, 2007), and for the non-multiferroic ME Cr_2O_3 (Chen *et al.,* 2006). Record high ME responses of stress-strain coupled composites like PZT/FeBSiC (Nan *et al.*, 2008) rather find applications in sensorics.

Double Perovskites: from half-metallic ferrimagnets to Mott-Hubbard insulators

J. Kübler

Theoretische Physik, Technische Universität Darmstadt, 64289 Darmstadt, Germany

juergen.kuebler@gmail.com

Certain double perovskites ($Sr_2B'B''O_6$, for B' = Cr or Fe and B'' 4d and 5d transition metal elements, and Ba_2MnReO_6 as well as Ba_2FeMoO_6) possess – with some noteworthy exceptions – fully spin-polarized ground states and are of possible interest for spintronics applications. Using the local spin-density functional approximation (LSDA), the GGA and LDA+U the electronic structure of this series of double perovskites will be discussed. Using the results from LSDA, GGA, and LDA+U calculations, together with a simple formula for the Curie temperature, T_C , we can explain an observed trend in the T_C's of this series of compounds. (*Work done in collaboration with Claudia Felser, Tapas Mandal, and Martha Greenblatt.*)

Experimental Procedure for Fabrication of Magnetic Tunnel Junctions and Recent Progress of TMR effect in Magnetic Tunnel Junctions

T. Kubota, G. Kim

Department of Applied Physics, Tohoku University, Sendai 980-8579, Japan

takahide@mlab.apph.tohoku.ac.jp
kim@mlab.apph.tohoku.ac.jp

Since the discovery of the tunnel magnetoresistance (TMR) effect,[1–3] the study of magnetic tunnel junctions (MTJs) has expanded quickly and widely. Various spinelectronics devices using MTJs are strongly expected to be fabricated in the future. Experimentally, micro-fabrication using lithography technique plays an important role in observation of TMR effect. In our group, MTJs are fabricated by using of conventional electron beam(EB)- or photo-lithography techniques and dry etching process by Ar ion milling.
In the first part of our talk, we will introduce how to make magnetic tunnel junctions using photo (or EB) - lithography technique. In the latter part, recent progress of TMR effect in magnetic tunnel junctions with Heusler compounds' electrodes and perpendicular magnets' electrodes will be discussed. As is generally known, Heusler alloys, especially Co-based compounds, are one of the promising half-metal ferromagnets and MTJs using such Heusler alloys exhibits Half-metallic behavior [See ref. 4].

Also, ferromagnetic materials with perpendicular magnetic anisotoropy have a potential to make a great progress in spin-electronics devices. Namely, for realizing the giga-bit-class MRAMs, minimization of the bit cells are required and thermal instability of the bits should be cared. To avoid the instability, ferromagnetic electrodes with *high* perpendicular magnetic anisotoropy, such as *L*10-ordred CoPt and FePt are desired as candidates of ferromagnetic electrodes in MTJs. We have succeed in fabricating MTJs with *L*10-CoPt and MgO tunneling barrier and observed 10%-TMR ratio at low temperature [5].

We will show some recent experimental results regarding MTJs with Co2MnSi Heusler alloy and perpendicularly magnetized *L*10-CoPt electrodes.

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NMR – Introduction and application to spin polarized Heusler compounds

S. Wurmehl

Physics of Nanostructures; Department of Applied Physics / Center for NanoMaterials; Eindhoven University of Technology; P.O. Box 513, 5600 MB Eindhoven, The Netherlands

S.wurmehl@TUE.nl

Nuclear Magnetic Resonance (NMR) is based on the interaction of the nuclear magnetization with the effective field present at the nucleus. However, in case of dia- or paramagnetic materials the effective field is mainly determined by external applied magnetic fields. In ferromagnetic (spin polarized) materials, the effective field is dominated by the hyperfine field. The hyperfine field is a unique probe of the direct local environments of the NMR active atom. This local character of NMR arises from local contributions to the hyperfine field, namely the transferred field which depends on the nearest neighbor atoms and their magnetic moments. This enables NMR to study the (local) structural properties of bulk samples as well as of thin films of spin polarized materials.

Materials with a high spin polarization at the Fermi-energy are interesting for a new research field: the spintronics. Spintronics combines the use of both the charge and the spin of an electron as information carriers, which promises distinct advantages over the conventional electronics which make only use of the charge of electrons. Particularly, half-metallic ferromagnets are a hot topic of many research groups, as they are predicted

to be 100% spin polarized, e.g. having electrons at the Fermi level with one single spin direction.
Heusler compounds are ternary intermetallic X_2YZ-compounds, crystallizing in the $L2_1$ structure. Among them are many ferromagnets which are predicted to be half-metallic. This is the reason why Heusler compounds are an interesting research topic in the field of spintronic materials.
A successful application of materials in spintronic devices requires a detailed knowledge of the interplay between the structure and the magnetic and electronic properties on an atomic scale. This is achieved by gaining knowledge of the local structure by means of NMR.
This talk will start with an introduction to the basics of NMR spectroscopy. In the following, recent results of structural characterization of spin polarized Heusler compound (such as bulk samples of Co_2FeAl, the substitutional series $Co_2Mn_{(1-x)}Fe_xSi$ and thin films of Co_2FeSi) will be discussed.

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