MA 37: Magnetic Semiconductors II

Time: Wednesday 14:45–16:45 Location: HSZ 401

MA 37.1 Wed 14:45 HSZ 401

Magnetic ordering in manganese stabilized zirconia — •Jan Zippel, Michael Lorenz, Jörg Lenzner, Anette Setzer, Pablo Esquinazi, and Marius Grundmann — Universität Leipzig, Institut für Experimentalphysik II, Linnéstraße 5, 04103 Leipzig

The selective control of the spin of electrons as a new degree of freedom in a conventional charge-based electronic offers the possibility to combine the advantages of non-volatility and fast data processing with the properties of conventional semiconductor devices. Recently, ferromagnetism has been observed in nominally undoped oxides like ZnO, HfO_2 or TiO_2 [1]. The origin of the observed ferromagnetism is still a controversy [2].

We present the growth of manganese doped zirconia (MnSZ) with pulsed-laser deposition (PLD). For Mn contents x>15 at%, we were able to stabilize MnSZ in its cubic crystalline phase being predicted to show ferromagnetic properties [3]. A weak, doping independent ferromagnetism in undoped as well as in manganese stabilized zirconia is observed. Hysteresis loops at $T = 5$K and at room temperature independent of x are shown. The lack of Mn induced magnetic ordering indicates, that the observed magnetic properties are defect related. The saturation magnetization at $T = 5$K depends on the strain as well as on the defect density of the films supporting the assumption of a defect related origin of the ferromagnetism.

[1] M. Khalid et al., Phys.Rev.B (2009), **80**, 035331 [2] M. Khalid et al., Phys.Rev.B (2010) **81**, 214414 [3] S. Ostanin et al., Phys. Rev. Lett. (2007) **98**, 016101

MA 37.2 Wed 15:00 HSZ 401

Magneto-optical studies on doped and undoped ZnO nanostructures — •Stephanie Jankowski[1], Limei Chen[1], Sebastian Geburt[2], Carsten Ronning[2], and Wolfram Heimbrodt[1] — [1]Department of Physics and Material Science Center, Philipps-University Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Physikalisch-Astronomische Fakultät, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, D-07743 Jena, Germany

High quality ZnO nanowires doped with different content of Manganese and Cobalt as well as ZnO quantum wells embedded between ZnMgO barriers are investigated by magneto photoluminescence and magnetic circular dichroism (MCD) in a split-coil superconducting magnet system. The measurements have been performed in magnetic fields up to 7 Tesla in a temperature range 1.6-300 K. MCD and Zeeman-spectroscopy in the excitonic region have been used to determine the g-factors of the samples. Even in case of transition metal doped ZnO surprisingly small Zeeman-splitting has been found. The reason for the rather small values as well as the change of sign of the g-value will be discussed. The transition metal doped ZnO shows also an interesting difference concerning the optical 3d intra-ionic transitions. Whereas in the Co-doped samples the 3d transitions are observable in case of the Mn-doped samples the Mn-PL is rather vanishing. The physical reasons for the odd behaviour will be discussed.

MA 37.3 Wed 15:15 HSZ 401

Magnetic properties of ZnO based diluted magnetic semiconductors using hybrid functional DFT — •Sanjeev K. Nayak, Heike C. Herper, Markus E. Gruner, and Peter Entel — Faculty of Physics, University of Duisburg-Essen, 47057 Duisburg

We study the magnetic properties of diluted magnetic semiconductor based on ZnO with transition metal dopants (Cr, Fe, Mn, Co and Ni) using the hybrid functional treatment in density functional theory (PBE0 [1], HSE [2]). At first the electronic structure using a semiconductor supercell is studied with the hybrid functional. Thereafter the dopants are substituted in the cation lattice sites, structurally relaxed and their magnetic properties are investigated. We mostly focus on the nearest neighbor interactions of the dopant atoms. Our preliminary results show that out of the two similar nearest neighbors (nn) in ZnO, the one lying along the c-axis favors a ferromagnetic alignment of Co spins and the other nn along the hexagonal plane favors antiferromagnetic interaction in GGA. However, both the nn separations stabilize antiferromagnetic interaction in hybrid functional calculations. This is similar to what is obtained when the Hubbard correlation U is added to the system. We compare the GGA+U and the hybrid functional results. All our studies are done with the Vienna ab-initio simulation package (VASP [3]).

[1] Paier *et al.*, J. Chem. Phys. **122**, 234102 (2005), [2] Paier *et al.*, J. Chem. Phys. **124**, 154709 (2006), [3] Kresse *et al.*, Phys. Rev. **B 54**, 11169 (1996)

MA 37.4 Wed 15:30 HSZ 401

muSR proof of magnetism in undoped ZnO thin films — •Thomas Tietze[1], Patrick Audehm[1], Boris Straumal[1,2], Peter Straumal[2], Zaher Salman[3], Hubertus Lütkens[3], Thomas Prokscha[3], and Eberhard Goering[1] — [1]Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart — [2]Moscow Institute of Steel and Alloys, Technological University, Leninsky Prospect 4, 119991 Moscow, Russia — [3]Paul Scherrer Institut, Labor für Myon-Spin Spektroskopie, CH-5232 Villigen PSI, Switzerland

Over the last decade tremendous efforts have been taken to reveal the origin of room temperature (RT) ferromagnetism (FM) in transition metal (TM) doped ZnO. SQUID measurements mostly showed ferromagnetic behavior whereas element specific methods like x-ray magnetic circular dichroism (XMCD) could not address the FM to any of the containing elements. FM occurred even in undoped ZnO, if the specific grain boundary area exceeds a threshold value. We suggest vacancy like states located at the grain boundaries as a possible source of the origin of RT FM of undoped ZnO. In order to proof intrinsic magnetism of nanostructured pure ZnO, we performed low energy muon spin rotation (LE-muSR) experiments at the Swiss Muon Source (SmuS). SQUID hysteresis loops revealed enhanced FM according to higher specific grain boundary area, in perfect agreement with our muSR measurements. The maximum muSR related magnetic volume fraction for nano grained samples was about 35%, while the pure ZnO single crystal sample was solely diamagnetic. Therefore, we present intrinsic evidence for a new type of RT-FM.

MA 37.5 Wed 15:45 HSZ 401

Defect induced ferromagnetic and metallic character of ZnO single crystals — •Khalid Muhammad[1], Pablo Esquinazi[1], Daniel Spemann[2], Wolfgang Anwand[3], and Gerhard Brauer[3] — [1]Division of Superconductivity and Magnetism, University of Leipzig, Germany — [2]Division of Nuclear Solid State Physics, University of Leipzig, Germany — [3]Institut für Strahlenphysik, Forschungzentrum Dresden-Rossendorf, Dresden, Germany

We investigated the magnetic and electrical properties of H-plasma treated ZnO single crystals. Hysteresis loops taken by SQUID magnetometry at 300 K showed a ferromagnetic behavior with a magnetization at saturation ~ 4 emu/g. A successive chemical etching process showed that the major ferromagnetic contribution comes from the first 10 nm layer. A clear semiconductor-metallic transition is observed in H-ZnO single crystals. The saturation magnetization as well as semiconductor-metallic transition temperature depend on the concentration of defects which is closely related to the exposed time of the sample to H-plasma. We observed a negative and positive magnetoresistance behavior. We attribute the ferromagnetic and metallic behavior of H-ZnO single crystals to hydrogen related defects.

MA 37.6 Wed 16:00 HSZ 401

Magnetic Properties of Polar ZnO Surfaces from *Ab-Initio* Calculations — •Guntram Fischer[1], Arthur Ernst[2], Waheed Adeagbo[1], Nadia Sanchez[3], Zdzislawa Szotek[4], Walter Temmerman[4], Wolfram Hergert[1], and Carmen Muñoz[3] — [1]University of Halle, Halle, Germany — [2]Max-Planck-Institute for Microstructure Physics, Halle, Germany — [3]Instituto de Ciencia de Materiales de Madrid, Madrid, Spain — [4]Daresbury Laboratory, Warrington, United Kingdom

We have investigated a magnetic moment formation of three oxygen-terminated polar ZnO surfaces. Specifically, these are the (000-1) surface, the (0001) surface with an oxygen atom on top of the Zn atom [(0001)-t], and the (0001) surface with an oxygen atom in a threefold hollow site [(0001)-h].

In this study we have used a multi-code approach allowing us to relax the surface structure and calculate the Heisenberg exchange parameters via a magnetic force theorem. Also, the influence of applying self-interaction corrections (SIC) to the oxygen p orbitals has been investigated.

Our calculations show that all three surfaces are magnetic. In addition, we find that applying SIC is necessary to correctly describe the top oxygen atom of the (0001)-h and (0001)-t surfaces, for both of which we find Curie temperatures to be larger than room temperature. The latter have been derived from Monte Carlo simulations based on the calculated exchange parameters.

MA 37.7 Wed 16:15 HSZ 401

F-centres and ferromagnetism in oxides — •Aurab Chakabarty and Charles Patterson — School of Physics, Trinity College Dublin, Dublin 2, Ireland

We present Hybrid and LDA calculations to explain the ferromagnetism (FM) observed in oxide thin films[1]. A model is proposed where FM can occur in oxides with F-centre defects when defect levels are partially filled and can be described by a single band Hubbard model. The model predicts room-temperature FM in large Hubbard-U limit[2]. We show that positively charged oxygen vacancy is metastable[3], but in oxygen poor and n-type conditions, oxygen and zinc vacancies are strongly bound together to form a ZnO divacancy, which is an F-centre with a Hubbard-U large enough to support ferromagnetism at room temperature. The Hubbard-U value is estimated from defect transition levels and from total energy calculations on divacancy pairs with parallel and anti-parallel magnetic moments. This model may also explain ferromagnetism in other nonmagnetic oxides such as MgO, as the MgO divacancy is an F-centre [4] with a large U.

References:
1. J.M.D. Coey et al, nat. mater. 4, 173 (2005)
2. J. A. Henderson et al, Phys. Rev. B. 46, 6328 (1992)
3. C. H. Patterson, Phys Rev. B, 74, 144432 (2006)
4. D. Ricci et al, J. Chem. Phys, 117, 2844 (2002)

MA 37.8 Wed 16:30 HSZ 401

Magnetism and correlation effects in "d^0" magnetic oxides — •Ivetta Slipukhina, Phivos Mavropoulos, Stefan Blügel, and Marjana Ležaić — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In the past few years there is a growing interest in engineering a ferromagnetic state in otherwise nonmagnetic insulators by doping with *sp* elements instead of transition metals that is traditionally used in diluted magnetic semiconductors. This novel magnetic materials design was stimulated by several unexpected experimental observations of room-temperature ferromagnetism in highly defective wide-gap semiconductors and insulators and is particularly interesting, both from fundamental and practical point of view. In this presentation we discuss possible d^0-magnetism in some otherwise non-magnetic oxides, using first-principles calculations within GGA and GGA+U approaches. Starting from Nitrogen doped MgO as a model system, we show that strong on-site electron interactions could lead to relative spin and orbital ordering of the Nitrogen induced hole states and significantly reduce the ferromagnetic exchange interaction. We discuss the mechanism behind the ferro- or antiferromagnetic state stabilization at different orbitally ordered configurations and analyze the influence of structural distortions on the magnetic interactions. The importance of structural distortions and strong electron correlations in Nitrogen doped $SrTiO_3$ perovskite is also examined. We gratefully acknowledge the support from HGF Nachwuchsgruppe Programme VH-NG-409.