MA 24: Magnetic Semiconductors

Time: Wednesday 14:45–19:15 Location: HSZ 401

MA 24.1 Wed 14:45 HSZ 401

Element specific structural and magnetic properties of Co-doped ZnO - from a paramagnet to a superparamagnetic ensemble — •Katharina Ollefs[1], Shuangli Ye[1], Verena Ney[1], Tom Kammermeier[1], Fabrice Wilhelm[2], Andrei Rogalev[2], and Andreas Ney[1] — [1]Fachbereich Physik, Universität Duisburg-Essen, Duisburg, Germany — [2]ESRF, Grenoble, France

The structural and magnetic properties of the dilute magnetic semiconductor (DMS) Co:ZnO prepared by reactive magnetron sputtering were studied using hard x-ray synchrotron radiation. By means of x-ray linear dichroism (XLD) measurements and respective simulations using the FDMNES code [1] the local crystallographic structure was investigated. For Co:ZnO with optimized growth conditions the local environment for both Co and Zn is the wurtzite structure of the ZnO bulk material. Virtually all Co dopant atoms are incorporated on cation lattice sites like previously shown for pulsed laser deposited samples [2]. X-ray magnetic circular dichroism (XMCD) and the corresponding element specific hysteresis at the Co K-edge reveal pure paramagnetic behavior as corroborated by SQUID measurements. Altered preparation conditions lead to the onset of phase-separation as revealed by a clear reduction of the XLD signal. With the onset of clustering a superparamagnetic blocking behavior arises which is typical for a particle ensemble. Changes in magnetic and electronic properties of such an ensemble due to annealing effects will be discussed.

[1] Y. Joly, Phys. Rev. B **63**, 125120 (2001)
[2] A. Ney *et al*., Phys. Rev. Lett. **100**, 157201 (2008)

MA 24.2 Wed 15:00 HSZ 401

Structural and Magnetic Properties of Gd doped ZnO — •Verena Ney[1], Fabrice Wilhelm[2], Tom Kammermeier[1], Shuangli Ye[1], Katharina Ollefs[1], Andrei Rogalev[2], and Andreas Ney[1] — [1]Experimentalphysik Universität Duisburg-Essen and CeNIDE, Lotharstr.1, D-47057 Duisburg, Germany — [2]European Synchrotron Radiation Facility (ESRF), 38043 Grenoble, France

The hope of discovering a dilute magnetic semiconductor (DMS) with ferromagnetic order up to room temperature still motivates research on suitable material combinations. Approaches with Co doped ZnO have shown that films with high quality show a purely paramagnetic behaviour [1], which turns to be superparamagnetic as soon as clusterformation starts. The comparison of ion-implanted Co:ZnO with Gd:ZnO showed that Gd might be a better candidate [2]. Therefore Gd doped ZnO was prepared by reactive magnetron sputtering with high concentrations ranging from 1.4% to up to 16% of Gd in ZnO. X-ray diffraction and element specific x-ray linear dichroism (XLD) were used for the structural characterization. The corresponding magnetic properties were measured with SQUID magnetometry and - again element specific - with x-ray magnetic circular dichroism (XMCD). Due to the large Gd-atom, the structural quality of the films is reduced with increasing Gd-content. Nevertheless, in the entire doping range we find no sign of intrinsic ferromagnetic interaction for the homogeneous Gd doped ZnO system as well as no long range magnetic order.

[1] A. Ney et al, Phys. Rev. Lett. **100**, 157201 (2008)
[2] V. Ney et al, J. Appl. Phys. **104**, 083904 (2008)

MA 24.3 Wed 15:15 HSZ 401

Room temperature ferromagnetism in carbon-implanted ZnO — •Shengqiang Zhou[1], Qingyu Xu[2], Kay Potzger[1], Juergen Fassbender[1], Manfred Helm[1], Holger Hochmuth[3], Michael Lorenz[3], Marius Grundmann[3], and Heidemarie Schmidt[1] — [1]Forschungszentrum Dresden-Rossendorf, Bautzner Landstraße 128, 01328 Dresden — [2]Southeastern University, Nanjing 211189, China — [3]Universität Leipzig, Linnéstraße 5, 04103 Leipzig

Transition metal (TM) doped ZnO has been extensively investigated due to its potential application as a diluted magnetic semiconductor with Curie temperature above room temperature. After one decade effort, however, the reported results are still very controversial concerning the reproducibility and the origin of the observed ferromagnetism. H. Pan et al. reported strong room temperature ferromagnetism in C-doped ZnO films grown by pulsed laser deposition [1]. Together with the first-principles calculations, evidence is given that carbon ions substitute for oxygen and their p-orbitals contribute the local magnetic moments. In this contribution [2], we introduced carbon into ZnO films by ion implantation. Room temperature ferromagnetism has been observed. Comparing with two reference samples, C implanted Ge and Ne implanted ZnO, which show only diamagnetism, our analysis demonstrates (1) the achievement of C-doped ferromagnetic ZnO by an alternative method, i.e. by ion implantation, and (2) the chemical involvement of carbon in the local magnetic moments is indirectly proven. [1] H. Pan et al., Phys. Rev. Lett. 99, 127201 (2007). [2] S. Zhou et al., Appl. Phys. Lett., arXiv:0811.3487 (2008).

MA 24.4 Wed 15:30 HSZ 401

Room temperature ferromagnetism without element specific ferromagnetism? A detailed XMCD study on doped ZnO — T. Tietze[1], M. Gacic[2], G. Schuetz[1], G. Jakob[2], S. Brück[1], A. Myatiev[3], B. Straumal[1,3], P. Straumal[3], and •E. Goering[1] — [1]MPI-MF, Stuttgart, Germany — [2]Institute of Physics, Johannes Gutenberg-University, Mainz, Germany — [3]Moscow Institute of Steel and Alloys, Moscow, Russia

On the quest for the intrinsic origin of ferromagnetism (FM) in ZnO doped with a few percent of nonmagnetic (d0) and magnetic transition metals, we present detailed XMCD measurements, performed in various detection modes to be sensitive to the surface, bulk, and interface related magnetism. The PLD prepared samples show strong FM at room temperature (RT) (SQUID: about 2muB/Co). On the other hand, XMCD at the Co L2,3 edges revealed only very small paramagnetic moments, while the Zn L2,3 and the O K edge measurements do not show any sign for magnetism at all. The Co L2,3 edge spectra reveal a multiplet like shape, which is clear evidence for Co located at the Zn site in a 3d7 configuration, also excluding metallic precipitates [1,2]. Therefore, we can exclude without doubt Co as a possible origin for FM in this system [2]. In addition, we have performed systematic investigations on the role of grain boundaries. These results strongly suggest grain boundary based vacancies, most likely at the oxygen site, as the source for the intrinsic RT-FM in doped ZnO. [1] M. Gacic et al., Phys. Rev. B 75 (2007) 205206 and APL 93 (2008) 152509 [2] T. Tietze et al., New Journal of Physics 10 (2008) 055009.

MA 24.5 Wed 15:45 HSZ 401

'Invisible' ferromagnetic secondary phases in Co doped ZnO — •Kay Potzger, Shengqiang Zhou, Arndt Mücklich, Qingyu Xu, Heidemarie Schmidt, Manfred Helm, and Jürgen Fassbender — Forschungszentrum Dresden-Rossendorf, Bautzner Landstraße 128, 01328 Dresden

The search for ferromagnetic transition-metal doped ZnO, i.e., diluted magnetic semiconductors (DMS), has turned into the search for unwanted secondary phases by high-resolution structural analysis [1]. Such phases even can lead to anomalous Hall effect arising from charge carrier spin polarization. In this talk we show that the general analysis technique for the identification, i.e. x-ray diffraction spectroscopy, fails to identify a recently observed kind of ferromagnetic inclusions with heavy crystalline disorder. We discuss the properties of those clusters using the popular Co:ZnO system.

[1] K. Potzger, S. Q. Zhou, H. Reuther, A. Mucklich, F. Eichhorn, N. Schell, W. Skorupa, M. Helm, J. Fassbender, T. Herrmannsdorfer, T. P. Papageorgiou, Appl. Phys. Lett. 88, 052508 (2006).

MA 24.6 Wed 16:00 HSZ 401

Magnetic phase of cobalt doped zinc oxide from first-principles and Monte Carlo methods — •Sanjeev kumar Nayak, Alfred Hucht, and Peter Entel — Physics Department, University of Duisburg-Essen, 47048 Duisburg, Germany

Understanding the magnetic properties of transition metal doped II-VI semiconductors, such as zinc oxide, is one of the active problems in materials science. Theoretically various mechanisms are sought to explain any underlying magnetic phenomena. Experimentally the situation is not yet conclusive. Hence, the need for thorough studies of this material is a priority. We studied the cobalt doped zinc oxide from a combination of different theoretical methods. The exchange interactions of cobalt spins in zinc oxide were calculated at various distances and for different compositions by the *ab-initio* technique. Treating the exchange interactions in a classical Heisenberg model, Monte Carlo simulations were done to study the phase diagram. Our results show no magnetization for doping concentrations below 20% cobalt. Inter-

mediate concentrations of cobalt doping sustain stable ferromagnetic phase, however, for large concentrations of cobalt, the system acquires a complicated phase with antiferromagnetically coupled ferromagnetic bi-layers. The Neél temperature of cobalt oxide from our calculations match very well with that of the experimental value for fcc lattice.

MA 24.7 Wed 16:15 HSZ 401

DMS GaMnN/AlGaN heterostructures — •Till Benter, Dong-Du Mai, Arne Urban, Joerg Malindretos, Michael Seibt, and Angela Rizzi — IV. Physikalisches Institut, Georg-August Universität Göttingen, 37077 Göttingen, Germany

GaMnN is a prototype GaN-based dilute magnetic semiconductor. Our earlier work showed only weak ferromagnetic coupling of single layer systems at room temperature with a saturation magnetisation of M_S = 0.025 μ_B/Mn and a small coercive field of 250 Oe, which leads to the assumption that only a small fraction of the incorporated Mn-ions participate in the ferromagnetic coupling. As an alternative system AlGaN/GaMnN/AlGaN heterostructures have been grown. The magnetization as well as the coercive field are strongly increased in these samples and the results are well reproducible. A TEM analysis exhibits regions of high Mn concentration at the upper heterojunction, which could be responsible for the coercivity. Mechnanical strain, polarization charges and diffusion barriers at the heterojunctions seem to influence the Mn incorporation into the GaN matrix. Diverse heterostructure configurations have been characterized concerning the magnetic and structural properties and the results are discussed with reference to the assumed double-exchange mechanism for the magnetic coupling.

MA 24.8 Wed 16:30 HSZ 401

Magnetization Control in Multifunctional Heterostructures — •M. Althammer[1], C. Bihler[2], W. Schoch[3], W. Limmer[3], R. Gross[1], M. S. Brandt[2], and S. T. B. Goennenwein[1] — [1]Walther-Meißner-Institut, Garching, Germany — [2]Walter Schottky Institut, Garching, Germany — [3]Institut für Halbleiterphysik, Ulm, Germany

The functionality of magnetoelectronic devices depends on the efficiency and scalabilty of magnetization control schemes. We here discuss the voltage control of magnetization orientation via the magnetoelastic channel in ferromagnetic semiconductor/piezoelectric actuator hybrid structures. The hybrids consist of a thin $Ga_{0.955}Mn_{0.045}As$ film cemented onto a piezoelectric actuator [1]. Using anisotropic magnetoresistance techniques, we have quantitatively determined the magnetic anisotropy within the plane of the $Ga_{0.955}Mn_{0.045}As$ films. Exploiting the substantial changes of the magnetic anisotropy in $Ga_{0.955}Mn_{0.045}As$ as a function of temperature T, different ratios between the magnetoelastic and the magnetocrystalline anisotropies can be realized in one and the same sample. At $T = 5$ K the magnetoelastic anisotropy term is only a small contribution to the total anisotropy, so that only the coercive fields are slightly modified as a function of the control voltage. For $T = 50$ K the magnetoelastic contribution dominates the magnetic anisotropy which allows to achieve a voltage control of the magnetization orientation by about 70°.

Financial Support by the DFG (SPP 1157, Li 988/4 and GO 944/3) is gratefully acknowledged.

[1] Bihler, *et al.*, PRB **78**, 045203 (2008)

MA 24.9 Wed 16:45 HSZ 401

On the formation of secondary phases in Fe implanted GaN — •Georg Talut[1], Helfried Reuther[1], Joerg Grenzer[1], Carsten Baehtz[1], Dmitri Novikov[2], and Bente Walz[2] — [1]Institute of Ion Beam Physics and Material Research, Forschungszentrum Dresden-Rossendorf e.V., P.O. Box 510119, 01314 Dresden — [2]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg

The request for room-temperature diluted magnetic semiconductors resulted in a large interest in GaN doped with transition metals. Recent investigations have shown that beside of the real dilute state spinodal decomposition as well as the formation of secondary phases may play an important role in the discussion of the origin of the ferromagnetism in GaN [1,2]. In this study, the formation of secondary phases was investigated in GaN epilayers deposited on sapphire and implanted with ^{57}Fe ions (3, 8 and 16×10^{16} cm^{-2}) at room temperature. Samples were annealed at 750° - 1200° C in N_2 and Ar flow for durations between some ms and some minutes. The formation of secondary phases in Fe implanted GaN upon annealing a N_2-flow was detected ex-situ by means of x-ray diffraction and Mössbauer spectroscopy and supported by SQUID magnetometry. During annealing in reduced N_2 atmosphere the reverse phase change from Fe_3N at room temperature to $Fe_{2.4}N$ at 1023 K was observed by means of in-situ x-ray diffraction. Samples, annealed by a flash lamp illumination in an Ar flow showed the formation of different secondary phases depending on annealing time and temperature. [1] Bonanni et al., PRL 101, (2008) 135502; [2] Li et al., Journal of Crystal Growth 310,(2008) 3294

MA 24.10 Wed 17:00 HSZ 401

Structural and magnetic properties of pulsed laser annealed GaMnAs — •Danilo Bürger[1], Mukesh Pandey[2], Shengqiang Zhou[1], Jörg Grenzer[1], Helfried Reuther[1], Wolfgang Anwand[1], Manfred Helm[1], and Heidemarie Schmidt[1] — [1]Institute of Ion Beam Physics and Materials Research, Forschungszentrum Dresden-Rossendorf, P.O. Box 510119, 01314 Dresden (Germany) — [2]High Pressure Physics Division, Bhabha Atomic Research Centre, 400085 Mumbai (India)

Magnetic semiconductors with high Curie temperatures T_C and large coercivity are very promising materials for spintronic applications. An approach to fabricate GaMnAs is the Mn-implantation of GaAs followed by pulsed laser annealing (PLA). We investigated the influence of Mn concentration and PLA conditions, e.g. number of pulses, pulse length, and pulse energy, on the structural and magnetic properties of GaMnAs. Using SQUID magnetometry, we revealed a strong decrease of the saturation magnetization with increasing number of pulses. HR-XRD-measurements revealed a lattice expansion normal to the surface after implantation. PLA leads either to a strain decrease (1 pulse) or even to a strain over compensation (10 pulses). We conclude that Mn implantation into GaAs followed by PLA is not sufficient for increasing the T_C in GaMnAs. In addition, the drawback of the Mn implantation is the loss of As from the GaAs surface as detected by means of Auger electron spectroscopy. Heat transfer calculations and coimplantation with suitable elements are possible approaches to enhance the properties of GaMnAs.

15 min. break

MA 24.11 Wed 17:30 HSZ 401

Ferromagnetism in $MgO_{1-x}N_x$: density-functional calculations — •Phivos Mavropoulos, Marjana Ležaić, and Stefan Blügel — Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

We examine the possibility of a magnetic state in Nitrogen-doped MgO. To this end, we discuss results of density-functional calculations within the Korringa-Kohn-Rostoker Green-function method in the coherent potential approximation for the description of disorder in $MgO_{1-x}N_x$ and within the pseudopotential method for structural relaxations. We find that, when Nitrogen is substituted in MgO, a spin-polarized impurity band emerges close to the MgO valence band, with a ferromagnetic state stabilized by the double-exchange mechanism. The Curie temperature, estimated within the random phase approximation with exchange constants calculated by the Liechtenstein formula, is found to increase linearly above a percolation threshold of $x \approx 2\%$, reaching 35 K at 10% and 90 K at 20% concentration. While for isolated substitutional impurities structural relaxation is insignificant, for dimers or trimers we find that it can lead to an insulating but still magnetic state. In the case of interstitial impurities we see that the O atom is pushed out of the ideal lattice position, forming a dumbell configuration around it together with the N atom. A pair of close-by N interstitials also push the two associated O atoms out of their lattice positions, resulting in a non-magnetic configuration.

MA 24.12 Wed 17:45 HSZ 401

Evidence for a magnetic proximity effect up to room temperature at Fe/(Ga,Mn)As interfaces — Francesco Maccherozzi[1], Matthias Sperl[2], Giancarlo Panaccione[2], Giorgio Rossi[1,3], Jan Minar[4], Svitlana Polesya[4], Hubert Ebert[4], Ursula Wurstbauer[2], Georg Woltersdorf[2], Werner Wegscheider[2], and •Christian Back[2] — [1]Laboratorio Nazionale TASC, INFM-CNR — [2]Fakultät für Physik, Universität Regensburg — [3]Dipartimento di Fisica, Universita di Modena e Reggio Emilia — [4]Department of Chemistry, Ludwig-Maximilians University Munich

The combination of Diluted Ferromagnetic Semiconductors (DMS) and conventional semiconductors promises electronic devices with new functionalities such as non-volatility and the additional spin degree of freedom. Here we demonstrate that the low Curie temperature of DMS can be increased by using ferromagnetic proximity polarization. We show that a thin layer of (Ga,Mn)As can be spin polarized at room temperature by the proximity to an iron overlayer. X-ray magnetic

circular dichroism and superconducting quantum interference device magnetometry are used to study magnetic order in the iron film and in (Ga,Mn)As films. We conclude that the induced magnetic order in the (Ga,Mn)As layer extends over more than 2 nm, even at room temperature. Furthermore, we show by experiment as well as by theory that the magnetic moments of the Mn ions are coupled antiparallel to the magnetization direction of the Fe layer. Our findings indicate that the ferromagnetic proximity polarization effect can be used to control the spin state of a thin DMS at room temperature.

MA 24.13 Wed 18:00 HSZ 401

Local mapping of anisotropy in individual (Ga,Mn)As micro and nanostructures — •Frank Hoffmann, Georg Woltersdorf, and Christian H. Back — University Regensburg, Germany

(Ga,Mn)As films show a superposition of various magnetic anisotropies which have different physical origins. Recently it was shown that the effective anisotropy can be altered significantly when the film is patterned into nanoscale elements [1]. For spin-injection and magnetotransport experiments with (Ga,Mn)As microstructures the knowledge of the magnetic ground state, the magnetic anisotropies and the switching behavior is crucial. By combining time-resolved Kerr microscopy and ferromagnetic resonance (FMR) we are able to perform local resonance and hysteresis measurements on individual nanostructures. The influence of strain on the magnetic anisotropies was investigated for two sample geometries. We observe a strong strain-relaxation induced uniaxial anisotropy with an easy axis parallel to the long edge for rectangular-shaped structures. Anisotropic relaxation of compressive strain in the (Ga,Mn)As stripes on a GaAs(001) substrate is the underlying mechanism for this behavior. In contrast our experiments on disk-shaped elements with laterally isotropic strain relaxation only show a lowering of the out-of-plane strain-induced anisotropy. These local changes of the magnetic anisotropy which take place at the boundary of the elements can be even imaged with our spatially resolved measurements.

[1] Wenisch et al., PRL 99, 077201 (2007)

MA 24.14 Wed 18:15 HSZ 401

Multifarious-magnetism in copper oxide nanostructures from first-principles — •Xiang-Yuan Cui[1], Aloysius Soon[1], Bernard Delley[2], Su-Huai Wei[3], and Catherine Stampfl[1] — [1]University of Sydney, Australia — [2]Paul Scherrer Institut, Switzerland — [3]National Renewable Energy Laboratory, USA

Driven by the ever-increasing demand for novel spin-dependent advanced materials, investigation of nanoscale magnetic materials is currently actively pursued. With the latest developments focusing more on magnetic semiconducting oxides, materials based on cuprous oxide, Cu_2O, are of high interest as potential *p*-type semiconducting candidates. Thus developing an understanding of how intrinsic defects influence both its electronic and magnetic properties is important.

We perform density-functional theory calculations[1] and analyze both the electronic and magnetic properties of native defects in both bulk Cu_2O and its surfaces, as well as their respective formation/surface energies under different growth conditions. We find that under oxygen-lean conditions, the experimentally observed ferromagnetic behaviour[2] could originate from copper vacancies on $Cu_2O(111)$ while under oxygen-rich conditions, low energy bulk oxygen interstitials might explain the ferromagnetic moment found in the same material. This suggests that the origin of observed magnetism in substoichiometric copper oxide nanoparticles could be multifarious, highlighting the complimentary role of bulk and surface native magnetic defects. 1. A. Soon *et al.* submitted, 2. A. Ye. Yermakov *et al.* J. Magn. Magn. Mater. **310**, 2102 (2007)

MA 24.15 Wed 18:30 HSZ 401

Strong electron correlation in transition-metal (TM) doped silicon crystals — •Frank Küwen[1], Roman Leitsmann[2] und Friedhelm Bechstedt[2] — [1]LaserAnwendungsCentrum, Technische Universität Clausthal, Am Stollen 19, 38640 Goslar — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena

A first priniciple investigation in density functional theory (DFT) has been made for TM doped silicon bulk crystals as well as for Si nanoparticles. Using the Vienna ab inito simulation package (VASP) we have calculated for relaxed geometries, single-particle energies, and magnetic moments in the spin-polarized generalized gradient approximation (GGA). The strong electron correlation has been taken into account through an effective Coulomb interaction via GGA+U and a non-local exchange-correlation potential within the Heyd-Scuseria-Ernzerhof (HSE) approach. The comparison of the resulting density of states (DOS) reveal significant influence of the strong electron correlation on the DOS, especially on the fundamental gap region, and hence on the total magnetic moments of the nanocrystals with TM atoms at different doping sites.

MA 24.16 Wed 18:45 HSZ 401

Impurity formation energies and effective interactions in DMS — Vaclav Drchal and •Josef Kudrnovsky — Institute of Physics, AS CR, Praha, Czech Republic

We use a recently developed method (Phil. Mag. 88 (2008), 2777) based on the TB-LMTO scheme to calculate the electronic structure of atomic clusters embedded in an ideal crystal or in an effective medium that represents a random alloy. We determine from the first principles impurity formation energies and effective interatomic interactions (i.e. the parameters of the alloy Ising Hamiltonian that governs structural stability of materials) and exchange interactions (i.e. parameters of the Heisenberg Hamiltonian that determines the magnetic structure). We will present the results for impurities in (Ga,Mn)As alloys and for vacancies and alkali metal impurities in zirconia that can induce the the so-called d0-magnetism.

MA 24.17 Wed 19:00 HSZ 401

Structural, chemical and magnetic characterization of epitaxial Fe on (Ga, Mn)As (001) — •Marcello Soda, Martin Utz, Werner Wegscheider, Josef Zweck, and Christian Horst Back — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Universitätstr. 31, 93053 Regensburg, Germany

An epitaxial Fe-film grown on the dilute magnetic semiconductor GaMnAs (001) induces antiferromagnetic coupling between the two materials at room temperature.

It is known that a 2 nm thick GaMnAs layer at the interface shows induced magnetic order at room temperature [1].

TEM analysis of the Fe/(Ga, Mn)As interface, in situ XPS measurements and MOKE measurements characterize the epitaxial quality and the magnetic properties of this material. TEM micrographs shows an epitaxial growth of Fe with a roughness of 2-3 monolayer confirming the good quality of the surface treatment. XPS measurements demonstrate the absence of intermixing between the two materials.

Finally MOKE curves of Fe/(Ga, Mn)As, compared to that of the as grown GaMnAs, demonstrate the superposition of the magnetic properties of Fe and GaMnAs.

[1] F. Maccherozzi et al. accepted for publishing on PRL