MA 12: Magnetic Particles/ Clusters II

Time: Monday 17:00–19:15 Location: HSZ 103

MA 12.1 Mon 17:00 HSZ 103

Structural and magnetic characterization of self assembled iron oxide nanoparticles — •Durgamadhab Mishra[1], Maria Jose Benitez[1], Philipp Szary[1], Giovanni A Badini Confalonieri[1], Mathias Feyen[2], Anhui Lu[2], Leonardo Agudo[3], Günther Eggeler[3], Oleg Petracic[1], and Hartmut Zabel[1] — [1]Festkörperphysik, Ruhr Universität Bochum D -44780 Bochum — [2]Max-Planck-Institut für Kholenforschung, D-45470 Mülheim an der Ruhr — [3]Institute of Materials, Department of Materials Science D-44780 Bochum

Magnetic nanoparticles (NPs) are at the forefront of research due to their potential in applications as e.g. in biomedicine, spintronics and high density data storage. Particularly iron oxide NPs have widely been investigated for their biocompatibility and half metallic properties. In order to achieve a complete control over the various functionalities one has to obtain well defined phases of iron oxide. We synthesized 20 nm NPs following the synthesis method as described in Park et al (2004). The NPs were self-assembled after spin-coating on Si substrates in monolayers or multilayers of NPs. Various annealing conditions lead to different iron oxide phases. We characterized the monolayers by grazing incidence diffraction (GID), SQUID magnetometry and dark field TEM analysis. We show that in all cases a multi-phase structure is obtained with finite exchange bias between a ferrimagnetic and an antiferromagnetic phase [1].

[1] M.J. Benitez et al., submitted (arXiv:1010.0938)

MA 12.2 Mon 17:15 HSZ 103

Fe oxide nanoparticles in dispersion measured by XAS — •Anne Warland, Carolin Antoniak, Masih Darbandi, Claudia Weis, Werner Keune, and Heiko Wende — Faculty of Physics and CeNIDE, University of Duisburg-Essen, Germany

Due to the wide range of biomedical applications like e.g., targeted drug delivery and hypothermia treatment, magnetic nanoparticles are the subject of intense research. Fe oxide nanoparticles are often used as contrast enhancers in the MRI. We investigated Fe_3O_4 (magnetite) nanoparticles as they are biocompatible and their surface can be functionalized. Magnetite consists of Fe^{3+} and Fe^{2+} ions in tetrahedral and octahedral lattice sites giving rise to a clear multiplet structure in the x-ray absorption spectrum at the Fe $L_{3,2}$ edges. We synthesized Fe oxide nanoparticles using a water-in-oil microemulsion technique, which yields nanoparticles with a narrow size distribution. Bare and silica coated Fe oxide nanoparticles of a core size of 7nm dispersed in ethanol have been investigated by means of x-ray absorption spectroscopy (XAS) allowing to disentangle the contributions of the Fe^{2+} and Fe^{3+} ions and therefore, to estimate the amount of Fe_3O_4 in the particles. Due to a special experimental setup (Liquidrom chamber)[1] provided at BESSY, the particles can be measured directly in dispersion. In case of the silica coated particles a high amount of magnetite was obtained. In contrast, the bare nanoparticles showed indications of further oxidation into Fe_2O_3. -Supported by DFG(SFB 445,WE 2623/3-1) and Helmholtz-Zentrum Berlin.

[1] Aziz Bekhit E F 2007, Dissertation FU Berlin.

MA 12.3 Mon 17:30 HSZ 103

Carbon-coated NiPt, CoPt nanoalloys: size control and magnetic properties — •A. A. El-Gendy[1,2], S. Hampel[2], A. Leonhardt[2], V. Khavrus[2], B. Buechner[2], and R. Klingeler[1] — [1]Kirchhoff Institute for Physics, University of Heidelberg, D-69120 Heidelberg, Germany — [2]Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Germany

Controlled synthesis of magnetic nanoparticles with well-defined size and composition is always a challenge in material-based nanoscience. Here, we apply the high pressure chemical vapour deposition technique (HPCVD) to obtain carbon-shielded magnetic alloy nanoparticles under control of the particle size. Carbon encapsulated NiPt, CoPt (NiPt@C, CoPt@C) nanoalloys were synthesized by means of HPCVD starting from sublimating appropriate metal-organic precursors. Structural characterization by means of high resolution transmission electron microscopy, energy dispersive x-ray analysis and X-ray diffraction indicated the formation of coated bimetallic NixPt100-x and CoxPt100-x nanoparticles. Adjusting the sublimation temperature of the different precursors allowed tuning the core sizes with small size distribution. In addition, detailed studies of the magnetic properties are presented. AC magnetic heating studies imply the potential of the coated nanoalloys for hyperthermia therapy.

MA 12.4 Mon 17:45 HSZ 103

Fabrication of ferromagnetic Co/Pt nanodots on NaCl-crystals — •Mahmut Cayliogl[1], Andreas Rathjen[1], Alexander Neumann[1], André Kobs[1], Andreas Meyer[2], Robert Frömter[1] und Hans Peter Oepen[1] — [1]Institut für Angewandte Physik, Universität Hamburg, Jungiusstr. 11, 20355 Hamburg, Germany — [2]Institut für Physikalische Chemie, Universität Hamburg, Martin-Luther-King-Platz 6, 20146 Hamburg, Germany

Recently, we have successfully studied the growth of ferromagnetic Co/Pt multilayers with perpendicular anisotropy on various substrates. Utilizing SiO_2 cores of micelles as shadow mask [1] we could create ferromagnetic nanodots in the range < 20 nm [2]. For the purpose of producing nanodots in solution we have investigated the growth and nanodot fabrication on NaCl. In this talk we report on the preparation of cleaved NaCl surfaces that is necessary to get a layer-by-layer growth of the multilayer and a monomicellar coverage via spin coating of the micelles. In contradiction to the results obtained with Si and SiO_2, multilayers of composition $(Co_{0,8nm}/Pt_{2nm})_4$ have an in-plane easy plane behavior. This indicates that the interface roughness is increased resulting in a reduced interface anisotropy. In the light of our proposed study we have also produced thicker single Co films sandwiched between Pt. Nanodots made of such films are ferromagnetic and could be dissolved in water and imaged via scanning electron microscopy.

[1] A. Frömsdorf (A.Meyer) et. al., Small **3**, 880 (2007),
[2] H.Stillrich et. al. Adv. Funct. Mat **18**, 76 (2008)

MA 12.5 Mon 18:00 HSZ 103

SP-STM study of bi-atomic Fe chains on (5×1)-Ir(001) — Matthias Menzel[1], Yuriy Mokrousov[2], Robert Wieser[1], Kirsten von Bergmann[1], Elena Vedmedenko[1], Stefan Blügel[2], Stefan Heinze[3], •Andre Kubetzka[1], and Roland Wiesendanger[1] — [1]Institut für Angewandte Physik, Universität Hamburg, 20355 Hamburg — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich — [3]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel

The magnetism of one-dimensional structures on surfaces has been a fascinating topic of recent theoretical research, but experimental investigations have struggled with difficulties, e.g. the low amount of magnetic material or the problem of surface intermixing [1].

Here we utilize the self organization of Fe atoms on the (5×1)-reconstructed Ir(001) surface to prepare bi-atomic Fe chains [2]. Scanning tunneling microscopy was performed at $T = 8$ K using spin-sensitive Cr and Fe coated W tips. We observe no magnetic contrast in zero magnetic field, while in fields applied perpendicular to the surface the chains exhibit a periodic pattern along their axis with a wavelength of three inter-atomic distances. In agreement with density functional theory calculations and Monte Carlo simulations we can show that the magnetic ground state of the Fe chains is a 120° spin-spiral which is stabilized in external fields while it fluctuates in zero field.

[1] D.H. Wei et al. Phys. Rev. Lett. **103**, 225504 (2009).
[2] L. Hammer et al. Phys. Rev. B **67**, 125422 (2003).

MA 12.6 Mon 18:15 HSZ 103

Ab initio energy landscapes including spin degrees of freedom — •Luis Enrique Diaz Sanchez, Junais Habeeb Mokkath, and Gustavo Pastor — Institut fuer theoretische physik, Universitaet Kassel, Heinrich Plett. Str. 40, 34132 Kassel, Germany

In this work we present a systematic performance analysis of spin-polarized-first-principles (SPFP) basin-hopping (BH) calculations. The global search and local minima are calculated in the framework of spin-polarized density functional theory within the generalized gradient approximation. This formalism allow us to identify not only low-energy isomers but also their respective magnetic properties. In order to explore the configuration space collective (or shake) moves and are employed. different magnitude of random displacements are considered. The variation of the magnitude of the random displace-

ments permit us to modulate the jumps into the different minima in the potential energy surface. Results for different initial configuration are presented: initial random-clusters created in the spirit of the big-bang method, present well know ground states geometries and configurations in which the atoms are also randomly large separated at the beginning. We will show that choosing a correct sett of move parameters the performance of the SPFP-BH is very good for small nanoalloys and that considering additional spin degrees of freedom it is possible to predict not only the most stable structural motifs, as it happens with the standard BH technique, but also isomers having different magnetic moments for the case of small FeCo composomers.

MA 12.7 Mon 18:30 HSZ 103

The role of bridge atoms in the ultrafast laser-driven spin-manipulation in charged magnetic two-center nanostructures — •Wolfgang Hübner[1], Chun Li[2], and Georg Lefkidis[1] — [1]University of Kaiserslautern and Research Center OPTIMAS, Germany — [2]Northwestern Polytechnical University, Xi'an, China

We present an *ab initio* theory of ultrafast laser-induced magnetic switching in charged magnetic two-center nanostructures via Λ processes [1-2]. To improve the spin transferability between the magnetic centers, and to fulfill the energetic requirements for the Λ process [3], a small number of bridge atoms (O and Mg) is inserted in order to connect the active magnetic centers (Fe, Co, Ni). The nature of these nonmagnetic bridges changes the overlap between the magnetic atoms. It is found that both types of bridges contribute to spin redistribution on magnetic centers, i.e. change the spin density or reverse the localization. Especially, in the spin-transfer scenario on [Fe-O(Mg)-Co]$^+$ the bridges improve the transferability between the magnetic centers due to the tilting or branching of the linear chain. We generally find that lowering the symmetry using bridging atoms facilitates spin transfer, while spin-flip depends basically on the nature of the magnetic center.

[1] C. Li, T. Hartenstein, G. Lefkidis, and W. Hübner, PRB **79**, 180413(R) (2009)
[2] C. Li, G. Lefkidis and W. Hübner, J. Phys.: Conf. Ser. **200**, 042014 (2010)
[3] G. Lefkidis, G. P. Zhang, and W. Hübner, PRL **103**, 217401 (2009).

MA 12.8 Mon 18:45 HSZ 103

Transition metal clusters deposited on graphene: a first-principles study — •Sanjubala Sahoo, Markus E. Gruner, and Peter Entel — Faculty of Physics, University of Duisburg-Essen, 47057 Duisburg

We have studied the structural and magnetic properties of clusters (Fe, Co, Ni, Pt)$_{13,55}$ supported on graphene. Our calculations are based on density functional theory (VASP). The structural stability of the metal clusters are studied both on a pristine (defect free) and a five-member ring graphene. The calculations show that, introducing a vacancy in graphene enhances the adsorption energy of metal clusters on the substrate. In addition, the catalytic behavior of transition metal clusters are studied through adsorption of carbon monoxide molecule on the transition metal clusters. The role of graphene in affecting the adsorption of carbon monoxide molecule on metal clusters will be presented.

MA 12.9 Mon 19:00 HSZ 103

Revealing the magnetization reversal mechanism - from coherent rotation in compact to domain wall propagation in fractal islands — •Alberto Cavallin[1], Fabian Natterer[1], Safia Ouazi[1], Géraud Moulas[1], Anne Lehnert[1], Stefano Rusponi[1], Stanislas Rohart[2], Wulf Wulfhekel[3], and Harald Brune[1] — [1]IPMC, École Polytechnique Fédérale de Lausanne (EPFL), Station 3-B, CH-1015 Lausanne — [2]Laboratoire de Physique des Solides, Université Paris XI et CNRS, F-91405 Orsay — [3]Physikalisches Institut, Universität Karlsruhe (TH), D-76131 Karlsruhe

Magnetic nanostructures grown by self-assembly at surfaces are ideal model systems to explore the ultimate density limit of magnetic recording. While is it generally accepted that the magnetic ground state of nanostructures with a size of a few thousand atoms or less is monodomain, i.e., all spins are ferromagnetically aligned to a single domain, the transition state reached upon thermally activated magnetization reversal as a function of the island size and shape is debated [1,2]. This state lasts only ps and there are no techniques to image it at this time scale with the required spatial resolution of sub-nm. Therefore it can only be inferred indirectly. Our combined magneto-optical Kerr effect (MOKE) and STM measurements reveal for Co islands on Pt(111) a shape-dependent transition from the coherent rotation of all spins to the nucleation and propagation of a domain wall, going from compact to fractal islands.

References: [1] M. Bode *et al.* PRL **92** 067201 (2004)
[2] S. Krause *et al.* PRL **103** 127202 (2009)