

MA 7: Joint Session "FePt Nanoparticles" (jointly with DS, MM), Organization: Michael Farle (Univ. Duisburg-Essen)

Time: Monday 15:00–17:45

Location: EB 202

Topical Talk MA 7.1 Mon 15:00 EB 202
Prediction of morphology-, composition- and size-related trends in FePt nanoparticles from first principles — ●MARKUS ERNST GRUNER — Faculty of Physics and Center for Nanointegration CeNiDE, University of Duisburg-Essen, 47048 Duisburg

Owed to the large magneto-crystalline anisotropy (MCA) of bulk FePt alloys, nanostructures with effective diameters as small as 4 nm are considered for ultra-high density recording applications. Structural defects as multiple twinning, segregation and partial ordering effectively reduce the MCA and thus severely limit the integration density. First principles calculations in the framework of density functional theory permit independent insight into the size-dependent interrelation between composition, structural stability and magnetism granting access to the electronic level. Site-resolved orbital moments and MCA are obtained a fully relativistic treatment including spin-orbit interaction.

Large scale calculations with up to 1415 atoms demonstrate that for diameters around 4 nm a close competition between multiply twinned and single crystalline morphologies is present, while the low energy of Pt surfaces enhances segregation. The systematic variation of 3*d* and 5*d* components reveals that especially addition of Mn can reduce twinning, while complicating the magnetic configuration. Structural and electronic changes which may degrade the magnetic properties must also be expected from a protective encapsulation with main group elements.

Topical Talk MA 7.2 Mon 15:30 EB 202
Coulomb Blockade effects in FePt nanoparticles — ●ARTUR ERBE¹, ULRICH WIESENHÜTTER¹, DARIUS POHL², BERND RELLINGHAUS², and JÜRGEN FASSBENDER¹ — ¹Helmholtz-Zentrum Dresden-Rossendorf — ²IFW Dresden

In order to correlate the size and crystallinity of FePt nanoparticles with their respective electrical and magneto-electrical properties individual nanoparticles are contacted using electron beam lithography. The particles are prepared from gas phase on electron transparent SiN membranes which allows the transmission electron microscopy of the same nanoparticle which is characterized electrically. The fabrication results in junctions, in which single FePt nanoparticles are connected to external leads. These junctions are tested electronically by measuring the current-voltage characteristics at various gate voltages, temperatures and magnetic fields. We observe Coulomb Blockade effects which are in agreement with the dimensions obtained from the TEM studies. The results of the magnetic nanoparticles are compared to measurements taken on Au nanoparticles of similar sizes.

Topical Talk MA 7.3 Mon 16:00 EB 202
Pt surface segregation and its impact on magnetism in FePt nanoparticles — ●ULF WIEDWALD — Institut für Festkörperphysik, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

The appealing magnetic properties of chemically ordered FePt alloys strongly depend on composition. In nanoparticles with diameters below 10 nm the relative number of surface-near atoms strongly increases, thus any tendency of segregation will significantly change the stoichiometry of the interior. As a result, magnetic moments as well as magnetic anisotropy may vary compared to the bulk. In the frame of the collaborative research center SFB 569 we prepared size-selected, hexagonally arranged metallic particles by precursor loaded reverse micelles and plasma etching [1]. Pt segregation [2] and its impact on magnetism were examined in-situ for naked, non-interacting FePt particles on Si/SiO₂ as function of size (2-10 nm) by photoelectron spectroscopy and x-ray magnetic circular dichroism. For partially L1₀-ordered particles we observe reduced spin moments with decreasing diameter while the orbital moment is found rather independent of size. As connected to the orbital magnetism, the effective magnetic anisotropy is also con-

served for decreasing diameters, though reduced relative to the bulk [3]. Reasons for these astonishing observations are discussed.

- [1] A. Ethirajan, U. Wiedwald, et al., *Adv. Mater.* 19, 406 (2007).
 [2] L. Han, U. Wiedwald, B. Kuerbanjiang, P. Ziemann, *Nanotechnol.* 20, 285706 (2009).
 [3] U. Wiedwald, L. Han, J. Biskupek, U. Kaiser, P. Ziemann, *Beilstein J. Nanotechnol.* 1, 24 (2010).

Topical Talk MA 7.4 Mon 16:30 EB 202
Understanding the Metal-Carbon Interface in FePt terminated carbon nanotubes — ●DARIUS POHL¹, FRANZISKA SCHÄFFEL¹, CHRISTINE TÄSCHNER¹, MARC H. RÜMMELI¹, CHRISTIAN KISIELOWSKI², LUDWIG SCHULTZ¹, and BERND RELLINGHAUS¹ — ¹IFW Dresden, P.O. Box 270116, Dresden, D-01171, Germany — ²Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

Plasma-enhanced chemical vapour deposition (PE-CVD) onto FePt catalyst films is used to synthesize carbon nanotubes (CNT) which are terminated with L1₀-ordered FePt nanomagnets with high magnetic anisotropy [1]. The CNT are characterized by means of low voltage aberration-corrected HRTEM. To gain a deeper insight into the growth mechanism and in order to understand the relative crystallographic orientation of the particles with respect to the CNT axes structural investigations are conducted with a strong focus on the atomically resolved characterisation of the FePt-CNT interface. An interface-near expansion of the metal lattice is observed and attributed to a segregation of Pt towards the surface of the catalyst particle. Detailed statistical HRTEM analyses of these interfaces reveal that the CNT preferentially emanate from {111} facets of the catalyst particle. Molecular dynamic simulations were conducted to estimate the desorption energy of carbon atoms for various surfaces. Our results indicate that the physical principle based upon which the interfacial metal facet is chosen is a reduction of the desorption energy for carbon [2].

- [1] F. Schäffel et al., *Appl. Phys. Lett.* 94 (2009) 193197.
 [2] D. Pohl et al., *Phys. Rev. Lett.* 107 (2011) 185501.

Topical Talk MA 7.5 Mon 17:00 EB 202
Atomistic characterisation of ultrahard nanomagnets — ●CAROLIN ANTONIAK — Experimentalphysik/AG Wende and Center for Nanointegration Duisburg-Essen (CeNiDE), Universität Duisburg-Essen, Lotharstr. 1, 47057 Duisburg

A combination of x-ray absorption spectroscopy (XAS) and density functional theory (DFT) has been used to study the magnetic properties like spin and orbital magnetic moments and effective magnetocrystalline anisotropy of chemically ordered FePt nanoparticles on an atomistic lengthscale. By choosing the appropriate capping material, these properties can be tuned between hard and soft magnetic with either high or low magnetic moments [1]. Focus of this talk will be the results of XAS allowing for an element-specific analysis of magnetic properties. Complemented with DFT calculations, it helps to gain more insight to the mutual influence of nanoparticles and capping material allowing to state design guidelines for improved materials which will be presented in this contribution.

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- [1] C. Antoniak, M.E. Gruner et al., *Nature Comm.* 2, 528 (2011)

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