MA 22: Magnetic Particles / Clusters II

Time: Wednesday 14:00–16:30 Location: H 1028

MA 22.1 Wed 14:00 H 1028

Magnetism in homonuclear 3d transition metal dimers — •Daniel Fritsch, Klaus Koepernik, Manuel Richter, and Helmut Eschrig — Leibniz Institute for Solid State and Materials Research IFW Dresden, PO Box 270116, D-01171 Dresden, Germany

We have investigated the structural and electronic properties of the 3d transition-metal dimers utilising the full-potential local-orbital program package FPLO [1] for the solution of the Kohn-Sham equations using the local spin density approximation (LSDA). Special emphasis has been laid on the magnetic properties of the transition-metal dimers which are obtained from spin polarised relativistic calculations. Since orbital moments are usually underestimated in these calculations we have additionally studied the influence of orbital polarisation corrections (OPC) on the orbital moments. Such corrections have been suggested by Eriksson *et al.* [2] and later in slightly modified form by Eschrig *et al.* [3]. The results will be compared with available experimental data and other theoretical investigations available in the literature.

[1] K. Koepernik and H. Eschrig, Phys. Rev. B **59**, 1743 (1999); http://www.fplo.de.

[2] O. Eriksson, M. S. S. Brooks, and B. Johansson, Phys. Rev. B **41**, 7311 (1990).

[3] H. Eschrig, M. Sargolzaei, K. Koepernik, and M. Richter, Europhys. Lett. **72** 611 (2005).

MA 22.2 Wed 14:15 H 1028

Chemical ordering and magnetic properties in bimetallic transition metal clusters — •Sanjubala Sahoo, Georg Rollmann, Alfred Hucht, and Peter Entel — Physics Department, University of Duisburg-Essen, Duisburg Campus, 47048 Duisburg, Germany

Ground state properties of binary Co-Mn icosahedral clusters are studied using the density functional theory. The structural and magnetic properties are studied with respect to various compositions of the constituents. Recent experimental observation of increase in the average magnetic moment of Co-Mn clusters with increase in Mn concentration is clearly reproduced in present studies and is related to the fact that for the smaller Co-Mn clusters with a total number of atoms, N $\leq$ 147, the Mn atoms are preferably embedded on the surface of clusters. In addition, results on Co-Fe, Co-Ni and Fe-Mn clusters will also be presented.

MA 22.3 Wed 14:30 H 1028

Tuning the magnetic properties of deposited transition metal clusters by decoration — •Jan Minar[1], S. Bornemann[1], H. Ebert[1], J.B. Staunton[2], S. Rusponi[3], and H. Brune[3] — [1]Dep. Chemie, LMU, Butenandtstr. 5-13, 81377 M\"unchen, Germany — [2]Department of Physics, University of Warwick, UK — [3]EPF Lausanne, Switzerland

Using the fully relativistic version of the KKR-method for electronic structure calculations within local spin density functional theory (LSDA) the magnetic properties of Fe, Co and Ni clusters deposited on the Pt(111) surface have been investigated. Of central interest are the role of spin-orbit coupling as it influences the spontaneous formation and orientation of magnetic moments and gives rise amongst others to the occurrence of orbital magnetic moments, the magnetic anisotropy energy (MAE) and magnetic circular dichroism in X-ray absorption (XMCD). Our systematic investigations of different clusters and nanostructures aim to reveal the mutual relationship among their spin-orbit induced properties. In addition they show how their various magnetic properties depend on the structural properties and chemical composition of the studied system. For large two-dimensional clusters we focussed especially on the dependency of the MAE on decoration with another transition metal. Our results are in qualitative agreement with recent experimental findings. We resolved the MAE contributions for inequivalent cluster atoms and will discuss the effect of the induced MAE within the Pt substrate.

MA 22.4 Wed 14:45 H 1028

Synthesis and Characterization of Magnetic Nanoparticles — •Sabrina Disch, Wiebke Sager, Raphaël Hermann, Günter Goerigk, and Thomas Brückel — Institut für Festkörperforschung, Forschungszentrum Jülich GmbH; 52425 Jülich

Magnetic nanoparticles are the object of intensive research both because of their possible applications *e.g.* in information storage, catalysis, medical imaging and owing to the interest in fundamental understanding of their magnetic properties. Magnetic nanoparticles, as compared to bulk materials, show unique physical properties such as superparamagnetism or enhanced anisotropy constants. Very little is known about the magnetization distribution within a single particle and magnetic correlations in ordered arrangements of such nanoparticles. In order to investigate such phenomena using scattering techniques, samples of highly monodisperse nanoparticles are required.

We developed a synthesis route for the preparation of cobalt nanoparticles with diameters below 10 nm, originally based on the reduction of $Co(AOT)_2$ in water-in-oil microemulsions [1]. Our water-free synthesis route yields nanoparticle dispersions that are stable against oxidation for weeks if stored in nitrogen atmosphere. Here, we report on the progress made in synthesis optimization as well as magnetic characterization of the as-synthesized particles. We will also present results from scattering experiments performed on cobalt nanoparticles and on highly monodisperse iron oxide nanoparticles [2].

[1] C.Petit, A.Taleb, M.Pileni; *J. Phys. Chem. B*, **1999**, *103*, 1805.
[2] J. Park, T. Hyeon; *Nat. Mat.*, **2004**, *3*, 891.

MA 22.5 Wed 15:00 H 1028

Synthese von Au-core/Co-shell Nanopartikeln — •Britta Vogel[1], Carsten Waltenberg[2], Inga Ennen[1], Harald Rösner[3], Peter Jutzi[2] und Andreas Hütten[1] — [1]Department of Physics, University of Bielefeld, D-33615 Bielefeld, Germany — [2]Department of Chemistry, University of Bielefeld, D-33615 Bielefeld, Germany — [3]Institute of Nanotechnology, Forschungszentrum Karlsruhe GmbH, D-76021 Karlsruhe, Germany

Eine interessante Anwendungsmöglichkeit von magnetischen Nanopartikeln besteht im Einsatz in lebenden Zellen. Dazu ist es notwendig, die Nanopartikel mit einer biokompatiblen und oxidationshemmenden Hülle zu versehen. Eine Möglichkeit dafür bietet die Umhüllung mit Gold. [1][2]

Es wurden Cobalt-Nanopartikel durch thermische Zersetzung von Co-Precursoren synthetisiert, auf denen Gold durch Zersetzung eines Au-Precursors abgeschieden wurde. Untersuchungen der Partikel mittels HRTEM, EDX und EFTEM ergaben, dass bei dieser Synthese zunächst legierte Co/Au-Partikel als Zwischenprodukt entstehen. Es konnte experimentell durch Auslagerungsuntersuchungen gezeigt werden, dass das metastabile Zwischenprodukt in ein Au-core/Co-shell Partikel im Gleichgewichtszustand übergeht. Zudem werden magnetische Eigenschaften dieser Partikel diskutiert.

[1] R.Shenhar, V.M. Rotello, Acc. Chem. Res. 2003, 36, 549. [2] M. Ch. Daniel, D. Astruc, Chem. Rev. 2004, 104, 293.

MA 22.6 Wed 15:15 H 1028

Influence of biaxial stress on the magnetic properties of cobalt nanoparticles — •Srinivasa Saranu[1], Ulf Wiedwald[2], Paul Ziemann[2], and Ulrich Herr[1] — [1]Institut für Mikro- und Nanomaterialien, Universität Ulm, 89081 Ulm — [2]Institut für Festkörperphysik, Universität Ulm, 89069 Ulm

Co nanoparticles with an average diameter of 25nm have been produced using an inert gas condensation technique. The particles were deposited on Si substrates and covered in situ with a 20nm Cu film. When the substrate coverage exceeds 5 %, the remanent magnetization along the in-plane direction was larger than that along the out-of-plane direction which is attributed to the dipolar interaction between the particles. For Co particles on Ta substrates, the effect of stress on the magnetic properties of isolated particles was studied. A thin film of phospholipids (DOPC) on the Ta substrate was used to avoid the agglomeration of the particles during deposition. The lipid layer was removed in an oxygen plasma, afterwards the particles were reduced to metallic Co again using a hydrogen plasma and subsequently covered with 20nm of SiOx. The effect of stress on the magnetic properties of these particles was studied by loading the Ta substrate with hydrogen. For 0.6% of strain in the Ta substrate, out-of-plane magnetization measurements showed an increase of the saturation field Hs and a reduction of the remanent magnetization. This indicates that 25nm cobalt nanoparticles have a positive magnetostriction. Support

by the Landesstiftung Baden-Württemberg is greatfully acknowledged.

MA 22.7 Wed 15:30 H 1028

Analysis of the ultra-fast in-flight heating of FePt nanoparticles. — •Elias Mohn, Darius Pohl, Ute Queitsch, Franziska Schäffel, Ludwig Schultz, and Bernd Rellinghaus — IFW Dresden, P.O. Box 270116, D-01171 Dresden,

FePt nanoparticles within a size range of 4-6 nm are prepared by DC magnetron sputtering in an inert gas atmosphere and subsequently ejected into high vacuum via differential pumping. The particles are subjected to a heat treatment in high vacuum (HV) prior to there deposition onto substrates. In contrast to earlier experiments at somewhat elevated pressures [1], the in-flight annealing of the particles is done optically, since conventional convective heating is not possible under HV conditions.

In order to determine the experimentally hardly accessible temperature of the particles, the thermal history of the particles is rather calculated from the interaction with the electromagnetic field along the flight path through the light furnace used for the in-flight annealing. The results obtained for the particle temperature are corroborated by experimental findings on the sintering of agglomerated particles.

The experiments reveal that the effect of the thermal treatment on both the structural and magnetic properties of the FePt nanoparticles strongly depends on the particles' crystal structure before the annealing.

[1] S. Stappert et al., J. Crystal Growth 252 (2003) 440.

MA 22.8 Wed 15:45 H 1028

Magnetic Anisotropy as Function of Particle Diameter in FePt Alloy Particles — Ulf Wiedwald[1], Luyang Han[1], Andreas Klimmer[1], Balati Kurbanjan[1], Lianchen Shan[1], Hans-Gerd Boyen[1], Kai Fauth[2], and •Paul Ziemann[1] — [1]Institut für Festkörperphysik, Universität Ulm, Germany — [2]Max-Planck-Institut für Metallforschung, Stuttgart, Germany

FePt alloy nanoparticles show huge magnetic anisotropy energy (MAE) in the chemically ordered $L1_0$ phase. The ordered phase is typically reached by annealing above 900 K starting from chemically disordered FePt nanoparticles [1]. The plasma-induced nucleation of metal salt loaded reverse micelles allows the formation of self-assembled regular arrays on top of various substrates. Employing the micellar preparation route, the particle separation can be tuned between 20-100 nm and, thus, agglomeration during annealing is fully suppressed [2]. We investigated the formation of the $L1_0$ phase as functions of annealing temperature and time for 3-10 nm FePt particles. The phase transformation is tracked by hysteresis loops at 11 K and 300 K. 9 nm particles are ferromagnetic at 300 K and a MAE of $1-2\cdot10^6 \mathrm{J/m^3}$ is found after annealing at T = 1000 K. Despite an increasing MAE as a function of annealing temperature is observed for particles smaller than 6 nm, those, however, remain superparamagnetic at 300 K.

[1] U. Wiedwald et al., Appl. Phys. Lett. **90**, 062508 (2007)
[2] A. Ethirajan et al., Adv. Mater. **19**, 406 (2007)

*New address: H.-G. Boyen, University of Hasselt, Belgium

MA 22.9 Wed 16:00 H 1028

Chemical trends in structure and magnetism of binary multiply twinned nanoparticles — •Markus Ernst Gruner, Antje Dannenberg, and Peter Entel — Fachbereich Physik, Universität Duisburg-Essen, 47048 Duisburg, Germany

Arrays of $L1_0$ ordered nanoparticles of near-stoichiometric FePt and CoPt with diameters down to 4 nm are considered as promising material for future ultra-high density recording media. However, with decreasing particle size, also multiply twinned structures like decahedra and icosahedra are frequently encountered in experiment (e. g., [1]). These structures, however, will not posses the required hard magnetic properties due to the different crystallographic orientations of the individual twins. Recent large scale ab initio calculations of FePt clusters with up to 2.5 nm in diameter [2] show that ordered multiply twinned structures are energetically preferred over $L1_0$ cuboctahedra. Within this contribution, we discuss from the electronic structure point of view the influence of chemical trends on the structural stability of the $L1_0$ phase obtained by variation of the $3d$ and the $5d$ element.

[1] Z. R. Dai *et al.*, Surf. Sci. **505**, 325 (2002); D. Sudfeld *et al.*, Mater. Res. Soc. Symp. Proc. **998E**, 0998-J01-06 (2007)
[2] M. E. Gruner, G. Rollmann, P. Entel, M. Farle (submitted)

MA 22.10 Wed 16:15 H 1028

The effect of topology, charge and magnetic field on the arrangement of FePt nanomagnets on bacterial S-layers — •Ute Queitsch[1], Anja Blüher[2], Michael Mertig[2], Ludwig Schultz[1], and Bernd Rellinghaus[1] — [1]IFW Dresden, P.O. Box 270116 D-01171, Germany — [2]MBZ, University of Technology Dresden, Budapesterstr. 27, Dresden, D-01069, Germany

Gas phase preparation has proven to allow for the preparation of $L1_0$-ordered FePt nanoparticles by in-flight annealing prior to the particle deposition. The regular arrangement of the statistically arriving particles has been shown to be accomplished by depositing onto bacterial surface layers (S-layers) of Bacillus sphaericus NCTC 9602 exhibiting p4 symmetry and a lattice constant of 12.5nm. Aiming at improving the regularity of the particle arrangement we have explored the nature of the interaction between the particles and their affinity sites on the S-layers. Therefore, we have systematically varied both the particle size and charge. Upon adapting the particle size to the size of the template features we observe a pronounced improvement of the regularity. Varying the particle charge resulted only in a minor effect. Hence apparently, the observed affinity originates from topographical effects rather than from electrostatical interactions. In addition, the degree of agglomeration becomes important at high particle densities. Here, applying an in-plane magnetic field during the particle deposition is observed to result in a pronounced decrease of agglomeration and subsequently in an improvement of the regularity at high particle densities.