MA 32 Magnetic Particles / Clusters

Time: Thursday 15:15–18:45 Room: HSZ 401

MA 32.1 Thu 15:15 HSZ 401

The Mackay transition in Fe clusters — •Georg Rollmann, Alfred Hucht, Markus E. Gruner, and Peter Entel — Theoretical Low-Temperature Physics, University of Duisburg-Essen, Lotharstr. 1, Campus 47048 Duisburg, Germany

Icosahedral (Ih) structures are commonly observed in small clusters and even nanoparticles consisting of, e.g., rare-gas or transition-metal atoms. Their particular stability compared to corresponding cuboctahedral (CO), fcc-like packings is often related to their lower surface energy. However, due to the presence of internal strain, they become unfavorable for larger particles, and therefore a crossover from Ih to CO geometries is expected to occur with increasing particle size. Both packings can be transformed into one another via the Mackay transition [1].

We have investigated the potential energy surfaces of Fe clusters with closed atomic shells within density functional theory in the generalized gradient approximation allowing for full relaxation of the atoms. For Fe_{13}, the CO geometry is not stable with respect to a Mackay transformation, resulting in an Ih ground state. However, in the case of Fe_{55}, the lowest-energy isomer found is neither Ih nor CO, but has a CO-like core and an Ih shell. We also find these shell-wise transformed structures to be especially stable for larger Fe particles.

[1] A. Mackay, Acta Crystallogr. **15**, 916 (1962)

MA 32.2 Thu 15:30 HSZ 401

Influence of temperature on the magnetic properties of clusters — •Svetlana Polesya[1], Sven Bornemann[1], Jan Minár[1], Voicu Popescu[1], Ondrej Šipr[2], and Hubert Ebert[1] — [1]LMU München, Dept. Physikalische Chemie, München, Germany — [2]Institute of Physics Acad. of Science, Prague, Czech Republic

We investigate the temperature-dependence of the magnetisation of free Fe clusters and of supported Co clusters on Pt(111) and on Au(111). Electronic and magnetic properties of these systems at T=0 K are calculated ab-initio via a scalar-relativistic multiple-scattering formalism. Exchange coupling parameters are then obtained from zero-temperature results and employed for describing magnetic excitations at finite temperatures within a classical Heisenberg Hamiltonian. In that way, one can interconnect ground-state and finite-temperature properties. The mean magnetisation and magnetic profiles of clusters was evaluated by the Monte Carlo method. We show how the magnetic profiles of clusters change if the temperature is varied and how the dependence of mean cluster magnetisation on the cluster size is influenced by the temperature. In particular it turns out that for small clusters the critical temperature in general does not increase monotonously with the cluster size.

MA 32.3 Thu 15:45 HSZ 401

Magnetic and spectroscopic properties of Ru and Mo clusters deposited on Fe(001) and Ni(001) — •Sven Bornemann[1], Jan Minar[1], Wilfried Wurth[2], and Hubert Ebert[1] — [1]Department Chemie, LMU München — [2]Institut für Experimentalphysik, Universität Hamburg

The fully relativistic spin-polarized KKR method has been used to study the magnetic and spectroscopic properties of small Ru and Mo clusters deposited on Fe(001) as well as Ni(001). For both substrates the results for the XMCD spectra and their connection with the spin- and orbital moments will be discussed on the basis of the so-called sum rules.

In line with recent X-ray absorption experiments a pronounced XMCD signal is found for the $M_{2,3}$-edge of the Ru dimer on Fe(001). However, for a single Ru adatom no XMCD signal is found in the experiment, while theory predicts a dichroic signal and a magnetic moment of 0.84 μ_B for a single Ru adatom on a Fe(001) surface. In order to understand this contradiction with experiment we also simulated a stepped surface and an incorporation of Ru into the substrate. As it will show, this geometrical situations lead to a strong change in the magnetic moment compared to that of an isolated adatom.

MA 32.4 Thu 16:00 HSZ 401

Magnetic spin and orbital moments of mass-filtered Fe nanoparticles deposited on Co/W(110) — •Armin Kleibert[1], Joachim Bansmann[2], and Karl-Heinz Meiwes-Broer[1] — [1]Institut für Physik, Universität Rostock, Universitätsplatz 3, D-18051 Rostock — [2]Abteilung Oberflächenchemie und Katalyse, Universität Ulm, Albert-Einstein-Allee 47, D-89069 Ulm

In this contribution we focus on the magnetic spin and orbital moments of large Fe nanoparticles with diameters between 6-10nm (i.e. 15.000-50.000 atoms per cluster) deposited on ultrathin Co films on W(110). The moments have been obtained from *in situ* measurements of the XMCD (X-ray magnetic circular dichroism) via TEY (total electron yield) and are corrected for self-saturation effects. HRTEM (high resolution transmission electron microscopy) images yield structural and morphological properties of the Fe nanoparticles. The particles show bulk-like magnetic spin moments being nearly independent of the particle size. However, the orbital moments are strongly enhanced when compared to the bulk and exhibit a pronounced increase when reducing the size of the particles. Analysing the data reveals that the enhancement of the orbital moments is most probably not restricted to the surface of the particles. Thus, even the inner parts of the particles may possess properties being different from the bulk. As possible mechanisms we suggest size- and shape-dependent surface strain as well as surface relaxations, both being able to modify the crystal lattice as well as the symmetry. Moreover, we expect a significant influence of the substrate on the properties of the particles.

MA 32.5 Thu 16:15 HSZ 401

Magnetic moments of mass-selected FeCo alloy clusters on Ni(111)/W(110) — •R.K. Gebhardt[1], A. Kleibert[2], J. Bansmann[2,3], F. Bulut[1], K.-H. Meiwes-Broer[2], and M. Getzlaff[1] — [1]Institute of Applied Physics, University of Düsseldorf, Germany — [2]Institute of Physics, University of Rostock, Germany — [3]Institute of Surface Chemistry, University of Ulm, Germany

FeCo-alloys yield the highest magnetic moments of all binary 3d-transition metal alloys, such as $Fe_{50}Co_{50}$ about 2,5 μB (Slater-Pauling-curve). We prepared $Fe_{56}Co_{44}$ clusters (5 - 6 nm diameter) using the arc cluster ion source (ACIS) working in a continuous mode. The clusters were mass-selected by an electrostatic quadrupole deflector and subsequently deposited on Ni(111)/W(110). We present X-ray absorption measurements recorded under different angles. The investigation of the X-ray magnetic circular dichroism (XMCD) allows us to determine element-specifically the magnetic spin- and orbital moments. Measurements of the magnetic moments of larger clusters (7,5 nm diameter) are in a good agreement with the theoretically expected values in the solid [1,2]. Furthermore, the absorption measurements permit an estimation of the stoichiometry. Comparison of the angle-dependent absorption spectra gives indication of the cluster shape. The relation between size and magnetic properties will be discussed.

[1] J. Bansmann and A. Kleibert, Appl. Phys. A **80** (2005) 957
[2] M. Getzlaff et al., Appl. Phys. A **82** (2006) 95

MA 32.6 Thu 16:30 HSZ 401

Superferromagnetic domains in granular multilayers observed by X-PEEM and transmission x-ray microscopy — •S. Bedanta[1], T. Eimüller[2], P. Fischer[3], W. Kleemann[1], D.- H. Kim[3], E. Amaladass[4], S. Cardoso[5], and P. P. Freitas[5] — [1]Universität Duisburg-Essen, D-47048 Duisburg, Germany — [2]Ruhr-Universität Bochum, D-44780 Bochum, Germany — [3]Lawrence Berkeley National Laboratory, Berkeley CA 94720, USA — [4]Max-Planck-Institut fur Metallforschung, 70569 Stuttgart, Germany — [5]INESC, Rua Alves Redol 9-1, 1000 Lisbon, Portugal

Due to interparticle interactions, a collective superferromagnetic domain state is encountered in non-percolated granular multilayers $[Co_{80}Fe_{20}(t_n)/Al_2O_3(3nm)]_{10}$, where t_n represents the nominal thickness of CoFe [1-3]. Based on x-ray magnetic circular dichroic element-specific contrast, photoemission electron microscopy (X-PEEM) and transmission soft x-ray microscopy (XM-1), both at ALS, Berkeley, proved successful to image superferromagnetic domains at different external applied fields. Stripe domains stretched along the easy in-plane axis, but exhibiting irregular walls and hole-like internal structures ("domains

in domains") are revealed by X-PEEM on a sample with t_n = 1.3nm. More compact domains with a few μm in size were imaged by XM-1 on a sample with t_n = 1.6nm. Their growth was recorded during magnetization reversal under near-coercive magnetic fields.

[1] W. Kleemann *et al.*, Phys. Rev. B **63**, 134423 (2001).
[2] X. Chen *et al.*, Phys. Rev. Lett. **89**, 137203 (2002).
[3] S. Bedanta *et al.*, Phys. Rev. B **72**, 024419 (2005).

MA 32.7 Thu 16:45 HSZ 401

Preparation and characterisation of L10-FePt nanoparticles in the gas phase. — •Olga Dmitrieva, Günter Dumpich, Jöchen Kästner, and Mehmet Acet — Experimentalphysik, AG Farle, Universität Duisburg-Essen, 47048 Duisburg

FePt nanoparticles with sizes between 5-10 nm are prepared by inert gas condensation using DC sputtering and subsequent flight-annealing through a furnace set to temperatures in the range 600°C 1200°C. Morphology and structure of the obtained nanoparticles depend on the nucleation pressure and annealing temperature. The process at a nucleation pressure of 0.5 mbar yields multiply twinned icosahedral particles, whereas at 1.0 mbar, polycrystalline nanoparticles are observed. The desired chemically ordered L10-phase with high magneto-crystalline anisotropy in some particles was detected using high resolution transmission electron microscopy (HRTEM). With the addition of nitrogen to the sputtering gas, the formation of the icosahedral structure is suppressed, predominantly single crystalline L10-ordered nanoparticles are formed. To verify the incorporation of nitrogen into the atomic structure, we use electron energy loss spectroscopy (EELS) and X-Ray absorption spectroscopy (XAS). Work supported by DPG (SFB445).

MA 32.8 Thu 17:00 HSZ 401

Enhanced orbital magnetism in oxide-free FePt nanoparticles — •C. Antoniak[1], K. Fauth[2,3], H.-G. Boyen[4], U. Wiedwald[4], F. Wilhelm[5], A. Rogalev[5], M. Spasova[1], J. Lindner[1], M. Acet[1], and M. Farle[1] — [1]Fachbereich Pysik, Universität Duisburg-Essen, Lotharstr. 1, D-47048 Duisburg — [2]MPI für Metallforschung, Heisenbergstr. 3, D-70689 Stuttgart — [3]Experimentelle Physik IV, Universität Würzburg, Am Hubland, D-97074 Würzburg — [4]Abteilung Festkörperphysik, Universität Ulm, Albert-Einstein-Allee 11, D-89069 Ulm — [5]European Synchrotron Radiation Facility, 6 Rue Jules Horowitz, B.P. 220, F-38043 Grenoble

Wet chemically synthesised $Fe_{50}Pt_{50}$ particles with a mean diameter of 6.3 nm deposited on a naturally oxidised Si substrate have been structurally and magnetically characterised. By a soft hydrogen plasma treatment, the oxide shell and the organic ligands surrounding the chemically disordered particles in the as prepared state were removed and pure metallic x-ray absorption and magnetic circular dichroism spectra were measured at both the Fe and Pt $L_{3,2}$ edges. After annealing for 30min at 600°C in a hydrogen atmosphere of 5 Pa, the coercive field increased by a factor of 6. This indicates the formation of the chemically ordered $L1_0$ phase and is accompanied by an enhancement of the orbital magnetic moment at the Fe sites by more than 300%, whereas the magnetic moments at the Pt sites remain largely unchanged.
This work was supported by the BMBF (05 ES3XBA/5), the ESRF, the DFG (SFB 445) and the EU (MRTN-CT-2004-0055667, SyntOrbMag).

MA 32.9 Thu 17:15 HSZ 401

Phase transformation of FePt nanoparticles from fcc to fct as probed by XMCD — •Ulf Wiedwald[1], Birgit Kern[1], Kai Fauth[2], Andreas Klimmer[1], Luyang Han[1], Hans-Gerd Boyen[1], and Paul Ziemann[1] — [1]Abteilung Festkörperphysik, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany — [2]Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, 70569 Stuttgart, Germany

FePt alloy nanoparticles show huge magnetic anisotropy energy in the chemically ordered $L1_0$ phase. The ordered phase is typically obtained by annealing at 600-800°C starting from fcc, chemically disordered FePt nanoparticles. Nowadays, wet-chemical approaches like the synthesis of ligand-stabilized colloidal particles or the plasma-induced nucleation of metal salt loaded reverse micelles allow the self-organized formation in regular arrays onto various substrates. Hereby, the colloidal approach gives short interparticle spacing of 2-3 nm and the heat treatment at elevated temperatures is likely to form unwanted larger agglomerates of particles. By employing the micellar preparation route, the particle separation can be tuned between 20-100 nm. These larger distances permit us to study the phase transformation towards $L1_0$ ordered particles without any agglomeration, loss of the array quality or magnetostatic coupling between particles. We investigated FePt nanoparticles (4 nm and 9 nm) with spacing of 28 nm and 64 nm by XMCD. The phase transformation is tracked by hysteresis loops at various temperatures. In case of 9 nm particles we observe a coercive field of μ_0H = 0.2 T at 340 K. The magnetic anisotropy rises by more than one order of magnitude due to annealing, while the total magnetic moment remains nearly constant.

MA 32.10 Thu 17:30 HSZ 401

Charge Transfer Controlled Magnetism of FePt Nanoparticles — •Balaji Gopalan[1], Christophe Stroh[1], Keir Foster[1], Christian Lemier[1], Raghavan Viswanath[1], Jörg Weissmüller[1,2], and Stefan Mangold[3] — [1]Institut für Nanotechnologie, Forschungszentrum Karlsruhe GmbH, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany — [2]Fachrichtung Technische Physik, Universität des Saarlandes, 66041 Saarbrücken, Germany — [3]Institut für Synchrotronstrahlung, Forschungszentrum Karlsruhe GmbH, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany

The effect of charge transfer between ligand and nanoparticles on the magnetic properties of monodispersed 2.0 nm FePt nanoparticles is studied. For this purpose, we have synthesized FePt nanoparticles covered by high fatty acid ligand (FePtCL), octadecanethiol (FePtSH), and oleic acid/oleylamine mixture (FePtOAc) as a series and the magnetic properties are compared. The superparamagnetic blocking temperature (T_B) are found to be 14, 11 and 7.5 K for FePtCL, FePtSH and FePtOAC samples respectively. The coercivity (H_c) values measured at 5 K are 3880, 4800 and 4000 Oe for FePtCL, FePtSH, and FePtOAC respectively. These differences suggest that the effective magnetic anisotropy constant (K_{eff}) is different for these samples. XANES Fe K pre-edge values of 7114.6 and 7115.4 eV are observed for FePtCL and FePtSH (reference Fe value is 7112.1 eV) indicating that Fe in 2(+) and 3(+) oxidation states respectively in these samples. A correlation between the observed oxidation states and the magnetic properties will be attempted.

MA 32.11 Thu 17:45 HSZ 401

Synthesis of magnetic nanoparticles with pronounced shape anisotropy and characterization via small angle X-ray scattering (SAXS) — •Frank Döbrich, Andreas Michels, Andreas Tschöpe, and Rainer Birringer — Universität des Saarlandes, Technische Physik, Geb. D2 2, 66041 Saarbrücken, Germany

Ferrofluids (FF) are stable colloidal suspensions of magnetic particles in a nonmagnetic carrier fluid. This fact renders a FF sensitive to an external magnetic field, which leads to a coupling of magnetic and rheological properties. For instance, it is expected that a dispersion of highly anisometric particles such as rods or chains reveals a large enhancement (compared to spherical particles) of the magnetoviscous effect, i.e. the increase of the FF's viscosity due to an externally applied magnetic field. This contribution reports on the synthesis of a highly anisometric FF containing stable chains of iron nanoparticles and on the microstructural characterization by means of transmission electron microscopy (TEM) and small angle X-ray scattering (SAXS). The SAXS measurements develop a pronounced anisotropy of the scattering pattern as a function of increasing external magnetic field. Evaluation of the radially averaged SAXS curves in terms of basic scattering functions is discussed.

MA 32.12 Thu 18:00 HSZ 401

Magnetoviscous behaviour of nanorod ferrofluids — •Dörte Junk, Christian Lang, Andreas Tschöpe, and Rainer Birringer — Universität des Saarlandes, 66123 Saarbrücken, Germany

We prepare shape-anisotropic iron particles in a magnetic-field-assisted forced flux aerosol reactor. On their way downstream the particles are coated with oleic acid and dispersed in a carrier fluid. As in conventional ferrofluids these rod-like particles behave as Brownian particles. Their morphology has been characterized by TEM and ac susceptibility measurements in a dc bias field. We find an average aspect ratio lying between 10 and 15; we will call such a complex fluid nanorod ferrofluid (nrod FF). The magnetoviscous effect of the nrod FF has been studied using a squeeze flow viscometer (piezoelectric axial vibrator) in the presence of a homogenous magnetic field. The comparison with conventional FF reveals a giant magnetoviscous effect.

MA 32.13 Thu 18:15 HSZ 401

Characterization of magnetic nanoparticles by combining magnetization, magnetorelaxometry, ac susceptibility and microscopic measurements — •Frank Ludwig, Erik Heim, and Meinhard Schilling — TU Braunschweig, Institut für Elektrische Messtechnik und Grundlagen der Elektrotechnik, Hans-Sommer-Str. 66, D-38106 Braunschweig, GERMANY

The MAgnetic Relaxation ImmunoAssay (MARIA) uses superparamagnetic nanoparticles as markers and is based on the different relaxation times and behaviour of bound and unbound magnetic nanoparticles (MNPs). A crucial point is that MARIA relies on the availability of functionalized MNPs with a proper size and narrow size distribution. We have investigated various commercially available Fe$_{3}$O$_{4}$ MNP samples with organic shell, either diluted in water or immobilized by freeze-drying, combining static M(H) curves, magnetorelaxometry (MRX), ac susceptibility as well as TEM and AFM measurements. Whereas the microscopic data reveal rather local information on size and shape of MNPs, the magnetic measurements provide integral information on their size and size distribution as well as on magnetic properties, such as anisotropy constant, saturation magnetization and Néel and Brownian relaxation times. Especially MRX using fluxgates is shown to provide more information on MNP properties than SQUID MRX since it allows one to record the whole magnetization and relaxation process of MNPs.

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MA 32.14 Thu 18:30 HSZ 401

Investigation of biological research issues with superparamagnetic nanoparticles by differential fluxgate magnetorelaxometry — •Erik Heim, Kai Pöhlig, Frank Ludwig, and Meinhard Schilling — TU Braunschweig, Institut für Elektrische Messtechnik und Grundlagen der Elektrotechnik, Hans-Sommer-Str. 66, D-38106 Braunschweig, GERMANY

A promising bioanalytical application of superparamagnetic iron oxid nanoparticles (SPIOs) is the Magnetic Relaxation ImmunoAssay (MARIA). Commonly SPIOs are used as a contrast agent in magnetic resonance imaging. In MARIA biological targets are specifically marked with SPIOs. Here the relaxation signal of magnetized SPIOs is measured. Magnetic nanoparticles have the advantages of being non-toxic, that they can be used in opaque medium and that they are suitable for homogeneous assays at the same time. For MARIA the ideal SPIOs are monodisperse with a core diameter of 20 nm. So far commercially available SPIOs are not optimized for MARIA. Therefore we fractionize and functionalize these ferrofluids. As a model system to study binding kinetics we use SPIOs functionalized with streptavidin and biotinilated binding partners.

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