MA 17: Magnetic Particles and Clusters (jointly with CPP, BP)

Time: Tuesday 9:30–13:00 Location: H22

Invited Talk MA 17.1 Tue 9:30 H22

Magnetometry to identify the origin of printed documents — •Anna S. Semisalova, Vladimir N. Nikiforov, and Nikolai S. Perov — Lomonosov Moscow State University, Faculty of Physics, Moscow, Russia

Counterfeiting of valuable documents is an increasingly serious problem. For example, diplomas and stock certificates are all the subjects of increasingly frequent and accurate counterfeiting efforts. Identification of the true source of printed documents is a challenging task [1]. Many methods such as chemical analysis, various types of spectroscopy and microscopy, require a special sample preparation which may lead to the destruction of parts of the documents. Magnetometry may provide a non-destructive technique to uniquely identify the source of documents printed by using inks or toners containing magnetic particles.

Here, we will present an overview of the magnetic properties of documents produced by different laser printers (Canon, HP, Lexmark, Kyocera). The magnetic behavior of laser printers toners were investigated by vibrating sample magnetometry. Magnetic parameters such as coercive field and magnetic moment were measured, compared and are shown to be a possible source for classification, differentiation and identification of toner powders. The investigation of magnetic properties of toners could be considered as a new surprisingly simple non-destructive approach to certify and identify certain printers, since the printer toners were found to vary with manufacturer. The practical applications for counterfeit analysis are discussed. 1. Scientific Examination of Questioned Documents, ed. by Kelly J.S., 2006.

15 min. break

MA 17.2 Tue 10:15 H22

Printable giant magnetoresistive devices — •Daniil Karnaushenko[1,2], Denys Makarov[1], Chenglin Yan[1], Robert Streubel[1,2], and Oliver G. Schmidt[1,2] — [1]Institute for Integrative Nanosciences IFW Dresden, Helmholtzstraße 20, Dresden, 01069 Germany — [2]Material Systems for Nanoelectronics Chemnitz University of Technology, Straße der Nationen 62, Chemnitz, 09107 Germany

The rise of printable electronics is mainly indebted to huge efforts in materials science to fabricate cost-efficient versatile electronic building blocks such as transistors, diodes and resistors. However, the fabrication of printable electronic sensors and contactless switches operating in combination with magnetic fields remains challenging, mainly due to the lack of appropriate sensing compounds at ambient conditions. The printable magnetic sensor would act as a contactless switch in a complex printed electronic circuit. For this purpose, magnetic sensors with high sensitivity operating at room temperature have to be developed as inks, pastes or paints. Here, we demonstrate the first printable magnetic sensor that relies on the GMR effect. The developed multicomponent magnetic ink containing GMR flakes and nonconductive binder can be easily applied on various substrates, such as paper, polymer and ceramic. The fabricated sensor exhibits a room-temperature GMR of up to 8%, which is sufficiently high to develop a complete printed electronic circuit that is able to respond to an external magnetic field, opening new application fields in the modern electronics.

MA 17.3 Tue 10:30 H22

Influence of the local atomic structure on the magnetic properties of particulate FePt-X films — •S. Wicht[1,2], V. Neu[1], L. Schultz[1,2], O. Mosendz[3], G. Parker[3], D. Weller[3], and B. Rellinghaus[1] — [1]IFW Dresden, P.O. Box 260116, D-01171 Dresden, Germany. — [2]TU Dresden, IFWW, D-01062 Dresden, Germany. — [3]HGST, 3403 Yerba Buena Rd, San Jose, CA-95135, USA.

FePt-nanoparticles are a promising materials candidate for recording media aiming at storage densities beyond 1 Tbit/in^2. High-resolution electron microscopy (HRTEM) and vibrating sample magnetometry (VSM) are used to correlate the structural and magnetic properties of highly textured particulate films of matrix-isolated $L1_0$ ordered FePt-X (X: Cu/Ag). Particle size distributions and orientations of the particles' magnetic easy axes with respect to their MgO seed crystals and the substrate plane are determined from planview and cross-sectional HRTEM. The texture spread of the [001] easy axes is found to be roughly 3^o and clearly larger than the misalignment of the MgO crystals. Atomically resolved characterization of the FePt-X/MgO interfaces shows that this discrepancy is due to the nucleation of the FePt-X growth at MgO step edges. In accordance with the structural data, remanence measurements reveal only a weak dipolar coupling among the spatially separated FePt-X nanomagnets, and the anisotropy fields of the films are $\mu_0 H_A = 8 - 9T$. Surprisingly, the *magnetic* texture width as determined from an analysis of the hard axis magnetization curves is found to be one order of magnitude larger than the texture spread of the [001] axes. Possible origins of this finding are discussed.

MA 17.4 Tue 10:45 H22

Structural and Magnetic Properties of FePt@MnO Heterodimer Nanoparticles — •Alice Klapper[1], Xiao Sun[1], Oleg Petracic[1], Ulrich Rücker[1], Oskar Köhler[2], Heiko Bauer[2], Wolfgang Tremel[2], and Thomas Brückel[1] — [1]JCNS-2 and PGI-4, Forschungszentrum Jülich GmbH — [2]Institute of Inorganic Chemistry and Analytical Chemistry, Johannes Gutenberg University Mainz

On the length scale of few nanometers, surface effects are not negligible and therefore play an important role for the magnetic behavior of nanoparticles. In this work we investigate the magnetic properties of so-called FePt@MnO heterodimer nanoparticles, which consist of two exchange-coupled spherical nanoparticles, i.e. a ferromagnetic FePt and an antiferromagnetic MnO particle. The dimer nanoparticles have been precharacterized with respect to their structural properties via small angle x-ray scattering (SAXS) and a form factor model for particles consisting of two spherical subunits could be verified. This model has been proven by the anomalous SAXS (ASAXS) technique. The magnetic properties dependent on the size of the nanoparticles have been investigated with ZFC and FC measurements, using SQUID magnetometry. The exchange coupling could be proven by an exchange bias in hysteresis measurements as function of temperature. To investigate the ordering phenomenon the samples under study have been deposited on silicon substrates and dried with different applied magnetic fields. The dried samples have been studied using SEM and a chiral ordering of the heterodimer nanoparticles has been observed.

MA 17.5 Tue 11:00 H22

Stability and Meta-stability of Clusters in a Reactive Atmosphere: Theoretical Evidence for Unexpected Stoichiometries of Mg_MO_x — •Saswata Bhattacharya, Sergey V. Levchenko, Luca M. Ghiringhelli, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin-Dahlem 14195, Germany

Applying genetic algorithm and replica exchange molecular dynamics in a cascade approach we calculate structure and composition of Mg_MO_x clusters at realistic temperatures and oxygen pressures. The cascade starts with force field and goes up to density functional theory with exact exchange plus correlation in the random phase approximation.[1] The stable compositions are identified using *ab initio* atomistic thermodynamics. We find that at realistic environmental conditions small clusters (M = 1-5) are in thermodynamic equilibrium when $x > M$. Non-stoichiometric clusters are found to have in general higher spin multiplicity than stoichiometric ones. This suggests a possibility of tuning magnetic properties by changing environmental conditions.

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[1] X. Ren, P. Rinke, C. Joas, and M. Scheffler, Invited Review: Random-phase approximation and its applications in computational chemistry and materials science. J. Mater. Sci. 47, 21 (2012).

MA 17.6 Tue 11:15 H22

Cycloidal spin-structures in Bismuth iron-oxide nanoparticles — •Joachim Landers[1], Soma Salamon[1], Werner Keune[1], Marianela Escobar[2], Doru Lupascu[2], and Heiko Wende[1] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE), University of Duisburg-Essen, Duisburg, Germany — [2]Institute for Materials Science, University of Duisburg-Essen, Essen, Germany

Bismuth iron-oxide ($BiFeO_3$, BFO) nanoparticles of various diameters d prepared by a wet chemical method were studied using Mössbauer spectroscopy to determine the influence of the particle size ($d \gtrapprox 50$nm) on the cycloidal spin structure observable in BFO bulk material. Mössbauer spectra were measured at several temperatures to determine the orientation of magnetic moments relative to the crystal axes. This can be analyzed by investigating the quadrupole level

shift, which was in good agreement to bulk references. Considering effects on the relative spectral intensities and the resulting effective (hyperfine) magnetic field, a model of the ideal cycloidal structure was used to simulate a theoretical spectrum consistent with experimental Mössbauer spectra measured at 4.2K in an applied magnetic field of about 5T. The combination of both methods verifies the presence of a 'bulk-like' spin structure, which is still stable in nanoparticles with a diameter of about 54nm.

15 min. break

MA 17.7 Tue 11:45 H22

Ab initio spin-dynamics for nanostructures with application to domain walls through a Co nanocontact — Laszlo Balogh[1], Laszlo Udvardi[1], Krisztian Palotas[1], •Laszlo Szunyogh[1], and Ulrich Nowak[2] — [1]Department of Theoretical Physics and Condensed Matter Research Group of the Hungarian Academy of Sciences, Budapest University of Technology and Economics, H-1111 Budapest, Hungary — [2]Department of Physics, University of Konstanz, 78457 Konstanz, Germany

To calculate the magnetic ground state of nanoparticles we present a self-consistent first-principles method in terms of a fully relativistic embedded cluster multiple scattering Greens function technique. Based on the derivatives of the band energy, a Newton-Raphson algorithm is used to find the ground-state configuration. An extension of the method to finite temperatures is also presented.

The method is applied to a cobalt nanocontact that turned out to show a cycloidal domain wall configuration between oppositely magnetized leads. We found that a wall of cycloidal spin structure is about 30 meV lower in energy than the one of helical spin structure. A detailed analysis revealed that the uniaxial on-site anisotropy of the central atom is mainly responsible to this energy difference. The huge uniaxial anisotropy energy is accompanied by an enhancement and anisotropy of the orbital magnetic moment of the central atom. By varying the magnetic orientation at the central atom, we identify various on-site anisotropy terms and also those due to higher order spin interactions.

MA 17.8 Tue 12:00 H22

The Anderson Impurity Model in Finite Systems: A Study of Chromium Impurities in Gold Clusters — •Konstantin Hirsch[1,2], Vicente Zamudio-Bayer[1,2], Andreas Langenberg[1,2], Markus Niemeyer[1,2], Bruno Langbehn[1,2], Thonmas Möller[1], Akira Terasaki[3,4], Bernd von Issendorff[5], and Julian Tobias Lau[2] — [1]Institut für Optik und Atomare Physik, Technische Universität Berlin — [2]Institut für Methoden und Instrumentierung der Forschung mit Synchrotronstrahlung, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH — [3]Cluster Research Laboratory, Toyota Technological Institute, 717-86 Futamata, Ichikawa, Chiba 272-0001, Japan — [4]Department of Chemistry, Kyushu University, 6-10-1 Hakozaki, Higashi-ku, Fukuoka 812-8581, Japan — [5]Fakultät für Physik, Universität Freiburg

A long standing problem in condensed matter physics is the interaction of a single magnetic impurity with a free electron gas resulting in interesting phenomena like the Kondo effect. In recent years substantial progress was obtained by studying atomic scale systems. Here we want to follow this approach and investigate the interaction of a single magnetic impurity with a finite free electron gas. $CrAu_n^+$ clusters serve as a model system. We can show that the size dependence of the local spin magnetic moment of $CrAu_n^+$ can well be described within in the Anderson impurity model, whereas the interaction of the localized impurity states with the electron bath of the gold matrix is governed by quantum confinement in the host, which is abscent in the corresponding bulk material.

MA 17.9 Tue 12:15 H22

Rotational dynamics of Ni nanorod colloids characterized by optical transmission and neutron scattering — •Philipp Bender[1], Albrecht Wiedenmann[2], Annegret Günther[3], Dirk Honecker[3], Andreas Tschöpe[1], and Rainer Birringer[1] — [1]Universität des Saarlandes, Saarbrücken, Germany — [2]Institut Laue Langevin, Grenoble, France — [3]University of Luxembourg, Luxembourg

With diameters below 42 nm, Ni nanorods are uniaxial ferromagnetic single-domain particles. When dispersed in a liquid matrix, alignment of their magnetic moments along an external magnetic field is achieved by a rotation of the entire particle. In time-modulated magnetic fields the switching dynamics depends on the viscous friction of the nanorods in the liquid matrix. Due to the anisotropic electrical polarizability optical transmission measurements can be used to detect the response of a colloidal dispersion of Ni nanorods to a rotating magnetic field. In particular, the rotational diffusion coefficient can be extracted from the phase shift between the periodic variation of the rotating magnetic field and the resulting oscillation in the optical transmission. In the present study Small Angle Neutron Scattering (SANS) is used in addition to the transmission of polarized light to experimentally determine the hydrodynamic interactions of Ni nanorods with the liquid matrix in a rotating magnetic field.

MA 17.10 Tue 12:30 H22

Magnetic correlations in 3D ordered nanoparticle assemblies — •Elisabeth Josten[1], Oleg Petracic[1], Ulrich Rücker[1], Artur Glavic[2], Valeria Lauter[2], Erik Wetterskog[3], German Salazar-Alvarez[3], Lennart Bergström[3], and Thomas Brückel[1] — [1]JCNS-2 and PGI-4, Forschungszentrum Jülich, Germany — [2]Oak Ridge Natl Lab, Quant. Cond. Mat. Div, Oak Ridge, TN 37831 USA — [3]Stockholm Universitet, Department of Materials and Environmental Chemistry, Stockholm, Sweden

Nanoparticle superlattices can be considered as novel type of materials with controllable electronic, optical and magnetic properties. Understanding the magnetic behavior of ordered nanoparticle arrays is an important step towards the controlled design of e.g. novel devices. We have studied γ-Fe2O3 nanocubes and nanospheres with a diameter $\approx$ 10 nm. The particles have been deposited on a Si substrate to form highly ordered superstructures (mesocrystals) using a drop casting method. Structural characterization has been carried out using SEM, AFM, TEM and GISAXS. Depending on the shape of the particles, the arrays show mesostructures with bct or fcc symmetry with relatively long structural correlation lengths of 2-10 μm. In order to investigate magnetic inter-particle correlations we have employed grazing incidence neutron scattering experiments in reflectometry mode at the JCNS-instrument TREFF at the FRM II in Garching and in GISANS mode at the Magnetism Reflectometer at the SNS in Oak Ridge. These experiments yielded the degree of magnetic correlation for the in-plane and out-of-plane directions at different applied fields.

MA 17.11 Tue 12:45 H22

***Ab initio* study of spin and charge dynamics on the homodinuclear complex $[Ni_2^{II}(L\text{-}N_4Me_2)(emb)]$** — •Wei Jin, Georgios Lefkidis, and Wolfgang Hübner — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Box 3049, 67653 Kaiserslautern, Germany

We present a first-principles investigation of spin and charge dynamics on the recently synthesized and characterized homodinuclear compound $[Ni_2^{II}(L\text{-}N_4Me_2)(emb)]$ [1,2]. By calculating the oscillator strengths of the optical transitions we find good agreement of the peak positions in our theoretical ground-state absorption spectra with experiment. Extending our previous work [1], we predict a *local* ultrafast spin-flip scenario induced by high-energy laser pulses with the participation of charge-transfer states that are identified by Mulliken analysis of the involved states.

Additionally, for the two transient electronic states observed spectroscopically, which are related to the two charge dynamics with different time scales, we also fully characterize them and identify their relaxation time differences by exploiting the selection rules. The proof-of-principle demonstration clearly shows the possible application of optical properties and paves the way to coherently manipulate and detect spin and charge dynamics on dinuclear or even on multinuclear complexes.

[1] G. Lefkidis *et al.*, J. Phys. Chem. A. **115**, 1774 (2011).
[2] W. Jin *et al.*, Phys. Rev. Lett., in press.