P.12.11.13

Spin Reorientation in Thin Au/Co/Au Films: *in-situ* XMCD and EXAFS Study

Elisabeth Holub-Krappe[a], C. Andersson[b], T. Konishi[c], O. Karis[b], H.-J. Maletta[a], D. Arvanitis[b], [a]*Hahn-Meitner Institut, Berlin, Germany.* [b] *Physics Dept., Uppsala University, Sweden.* [c]*Chemistry Dept., Chiba Univerisity, Japan.* E-mail: holub-krappe@hmi.de

The preferred in-plane orientation of the magnetization in Co thin films can be switched to out-of-plane either by decreasing the thickness of the Co layer at fixed temperature, or the thickness of the Au cap layer, or by decreasing the temperature at fixed layer thickness. Recently, we have characterized the Co/Au system grown *in-situ* on a W(110) single crystal and found a novel behaviour, where a SRT can be observed over a wider range of Co thicknesses, depending on temperature and cap-thickness. Furthermore, we found a competing situation where the system was possible to stabilize both with an in-plane and an out-of-plane remanent magnetization for very thin Co layers. Our recent *in-situ* XMCD work indicates (a) for thick Co films the magnetization remained fully in-plane upon capping with Au, for all Au cap thicknesses. In the thin limit of Co thickness (case b) immediately after capping with Au the magnetization turned fully out-of-plane, and the overall magnetization increased upon further adding of Au. XMCD results will be discussed regarding the magnitude of magnetic moments, and especially on how the orbital moment varies in all cases which we studied. In short our results indicate that in the case (a) no variation of the orbital moment took place upon reorientation, in contrast to case (b). These observations reveal a more subtle dependence of the magnetic energies on the real space structure and add novel possibilities in order to create novel canted magnetic phases not observed earlier by tuning the growth parameters of this system, beyond what is reported in the literature.

Keywords: magnetic films, X-ray magnetic circular dichroism, XAFS

P.12.12.1

The Influence of Thermal Annealing on Magnetostatic Properties of Thin Fe and Ni Films

Edmunds Tamanis[a], E.E. Shaligina[b], L. Kozlovsky[a], [a]*Department of Physics, Daugavpils University, Latvia.* [b]*Department of Physics, University of Moscow, Russia.* E-mail: fizika@dau.lv.

Magnetic thin films exhibit unique physical properties, which allow to use them in the form of useful inventions [1-3]. The results of the investigation of the magnetostatic properties of the as-deposited and *in situ* annealed at temperature 573 K, 673 K and 773 K Fe and Ni films will be presented. The variations of the magnetic properties are analyzed as function of the film thickness, microstructure and surface roughness.

The dependance of the coercivity for the annealed samples was revealed. The observed variations of the magnetic properties as functions of thickness and annealing temperature were explained by the structural changes of the annealed Fe, Ni films in comparison with the as-deposited ones. In the case of Fe films the texture changes and K_α doublet resolution for thick films were found due to thermal recrystallization The marked distinction of the near-surface and volume magnetic characteristics of the Ni films was discovered. That was ascribed to both the distinguishing domain structure of the near-surface area and the film volume and the existing roughness at the film surface**.** The obtained new experimental data can promote further designing multilayered systems for modern devices of spin microelectronics.

[1] Xu M., Liakopoulos T.M., Ahn C.H., Han S.H., Kim H.J., *IEEE Trans. Magn.* 1998, **34** (4), 1369. [2] Kryder Y.M.H., *Thin Solid Films*, 1992, **216** (1), 174. [3] Lessoff H., Webb D. C., *Thin Solid Films*, 1976, **39**, 185.

Keywords: thin films, magnetic properties, annealing

P.12.13.1

Hydrophobic Drug Aggregates: Structure and Biology

Yulia Volovik Frenkel[a], Kalyan Das[a], Arthur D. Clark[a], Paul J. Lewi[b], Eddy Arnold[a], [a]*Center for Advanced Biotechnology and Medicine, and Department of Chemistry and Chemical Biology, Rutgers University, Piscataway, NJ, USA.* [b]*Janssen Pharmaceutica NV, Vosselaar, Belgium.* E-mail: yuliav@cabm.rutgers.edu

Using a variety of physicochemical approaches, we have determined that some highly hydrophobic drugs with great promise for the clinical treatment of AIDS form aggregated structures in simple aqueous solutions mimicking gastrointestinal conditions [1]. Aggregate size and oral bioavailability are correlated; compounds forming aggregate structures with 30-100 nm in radii had good bioavailability and those with aggregate sizes exceeding 250 nm in radii had poor bioavailability. The aggregates contain on the order of 10^6 drug molecules, with size depending on the structure of the compound and the solution conditions.

In the current study we have been exploring the structure and mechanisms of formation of NNRTI aggregates using diffraction, spectroscopic, and computational simulation approaches. The aggregates appear to represent an intermediate state between monomeric and precipitated forms of the hydrophobic compounds. X-ray powder diffraction measurements from the aggregates using synchrotron radiation at CHESS provided evidence for the presence of micro-crystalline domains. From our findings we are hoping to deduce an explanation of the unique biological behavior of these compounds.

[1] Frenkel Y.V., Clark A.D., Das K. Jr., Wang Y.-H., Lewi P.J., Janssen P.A.J., Arnold E., *J. Med. Chem*., 2005, *in press*.

Keywords: nanoparticles, pharmacology, microcrystalline domains

P.12.13.2

A First Principles Study of Stacking Fault and Surface Energies in Magnesium

Andrew E. Smith, Steven Homolya, *School of Physics and Materials Engineering, Monash University, Victoria 3800, Australia.* E-mail: andrew.smith@spme.monash.edu.au

Stacking fault and surface energies have been calculated for the basal and prismatic plane in magnesium using the first-principles ABINIT code. [1]

In extension of work by Uesugi et al. [2] calculations are presented for intrinsic, extrinsic and twinned stacking fault structures using the supercell approach [3]. Accordingly the generalized stacking fault energy is determined which represents the energy variation as a function of displacement of the crystal fault.

In order to achieve appropriate convergence of the energy calculations it is necessary to calibrate by determining the surface properties e.g. the surface energy, work function etc. [4]. In particular, the present work shows how careful choice of computational parameters avoids the usage of the somewhat spurious, in the present case, surface dipole correction.

[1] Gonze X., et al., *Comput. Mat. Sci*., 2002, **25**, 478-492. (The ABINIT code is a common project of the Université Catholique de Louvain, Corning Incorporated, and other contributors. See http://www.abinit.org.) [2] Uesugi T., Kohyama M., Kohzu M., Higashi K., *Mat. Sci. Forum*, 2003, **419-422**, 225-230. [3] Chetty N., Weinert M., *Phys. Rev. B*, 1997, **56**, 10844-10850. [4] Wachowicz E., Kiejna A., *J. Phys.: Condens. Matter*, 2001, **13**, 10767-10776.

Keywords: ab-initio calculations, stacking faults, energy calculations