O 60: Symposium: Bimetallic Nanosystems: Tuning Physical and Chemical Properties I (Invited Speakers: Harald Brune, Michael Hilgendorff, Konstantin Neyman)

Time: Thursday 9:30–12:15 Location: MA 005

Invited Talk O 60.1 Thu 9:30 MA 005

Interface *vs.* Alloy Contribution to Magnetic Anisotropy in Bi-Metallic Nanostructures — •Harald Brune — Swiss Federal Institute of Technology (EPFL), Lausanne, Switzerland

We investigate the magnetic anisotropy of atoms located at atomically sharp interfaces between two metals and of those situated in a homogeneous alloy. The numbers we derive enable to estimate whether homogeneous alloys or onion type alternations of two metals lead to higher anisotropies for a given size. The model systems are two-dimensional bi-metallic islands on Pt(111). The magnetic properties are determined by means of magneto-optical Kerr effect for island ensembles for which the morphology is derived from STM.

The blocking temperature of Fe_xCo_{1-x} alloy islands is highest for $x = 0.5$ and with $T_b = 160$ K two times higher than the one of pure Co ($T_b = 90$ K) or pure Fe islands ($T_b = 80$ K) of identical size and shape. This yields to an alloy contribution to the barrier for thermally induced magnetization reversal of $E_{alloy} = 0.14$ meV/atom. Co-core–Fe-shell islands reveal a steep increase of T_b, starting with minute amounts of Fe and ending at a shell being only 2 atomic rows wide. Further addition of Fe leads to a much more shallow increase of T_b, similar to the one of pure Fe or Co. From this behavior we infer that the interface between Co and Fe contributes by $E_{int} = 0.9$ meV/pair. These values suggests that abrupt 1D interfaces between two metals have significantly higher anisotropies than homogeneous alloys. For Co islands decorated by Pd we find very different anisotropies for lateral compared with vertical interfaces.

Invited Talk O 60.2 Thu 10:00 MA 005

Magnetic-Noble Metal Nanocomposites with Size-Dependent Magnetic Properties and Morphology-Dependent Optical Response — •Michael Hilgendorff — caesar research center, Bonn, Germany

This talk aims at presenting the preparation and the properties of bimetallic magnetic AgCo, PtCo, and PdCo core/shell nanocrystals and Au-CoPt3, Ag-CoPt3, and Au-FePt heterodimers.

Stable bimetallic AgCo, PtCo, and PdCo core/shell colloids with a narrow particle size distribution and a controlled shell-thickness have been obtained in organic solvents (toluene, diethylether or dioctylether) by means of wet chemistry. All three bimetallic particle systems are ferromagnetic at low temperatures and superparamagnetic at room temperature. Coercivity, blocking temperature, and oxidation stability depend on the thickness of the Co-shell.

The bimetallic heterodimers have been prepared by a seeded-growth approach in the presence of a cationic surfactant (cetyltrimethylammonium bromide, CTAB). Hydrophobic CoPt3 and FePt nanoparticles were transferred into water using CTAB as a phase-transfer agent and were subsequently used as seeding materials for the reduction of gold and silver precursors to produce the nanocomposites. Through the modification of the growth conditions, Au-CoPt3 nanocomposites with various morphologies (spheres, cubes, rods) were prepared, providing an opportunity to tailor the optical response of these composite nanoparticles while maintaining the magnetic properties of the original seeds, even upon phase transfer into water.

Invited Talk O 60.3 Thu 10:30 MA 005

Density functional studies of bimetallic nanosystems — •Konstantin Neyman — ICREA, Dept. de Química Física & IQTCUB, Universitat de Barcelona, Barcelona, Spain

Impressive progress in the computer performance together with drastically increased software efficiency has been recently achieved. This enabled computational studies of building blocks of metallic nanostructures that contain ˜100 (and more) atoms, thus approaching dimensions of the species dealt with experimentally, to be performed almost routinely using accurate density functional methods. In this way, even more complex nanosystems consisting of more than one metal also became treatable at this high computational level.

Opportunities for density functional calculations of bimetallic nanosystems will be discussed and the present status of the theoretical research in the field will be overviewed in the talk. Examples will be provided to illustrate effects of the second metal M in bimetallic nanoparticles and thin films Pd(1-x)M(x), (M = Zn, Ag, Au) on the adsorption properties and surface reactivity. Adsorbate-induced restructuring of bimetallic surfaces will also be addressed.

O 60.4 Thu 11:00 MA 005

Irradiation effects in FePt nanoparticles — Michael Müller and •Karsten Albe — Institut f. Materialwissenschaft, TU Darmstadt, Petersenstr. 23, D-64287 Darmstadt

FePt nanoparticles are a promising candidate material for ultra high density data storage because of their huge magnetic anisotropy energy in the chemically ordered L1_o phase (fct). Particles can be prepared in ordered arrays, but are mostly disordered and also occur in multiply twinned configurations. Since thermal annealing leads to a destruction of the patterned arrays, alternative methods are needed to transform the particles into the thermodynamically stable single crystalline ordered phase. In this contribution we use atomic scale computer simulations in order to study the possibility of structural modification and enhanced ordering of L1_o nanoparticles by ion irradiation. Molecular dynamics simulations are used to investigate defect production and sputtering as well as phase transformation processes in twinned and single-crystalline nanoparticles. Lattice-based Kinetic Monte Carlo simulations are employed in order to study the influence of athermal vacancies on the ordering kinetics. We compare the case of He-irradation at low and elevated temperatures while taking into account defect production and sputtering yields as obtained from our MD-simulations.

O 60.5 Thu 11:15 MA 005

Non-Intensive Phase Diagrams of Pt-Rd Nanoalloys — Johann Pohl, •Karsten Albe, and Mathias Nalepa — Institut f. Materialwissenschaft, TU Darmstadt, Petersenstr. 23, D-64287 Darmstadt

We present computer simulation studies on size dependent phase diagrams of Pt-Rh nanoparticles, which exhibit ordered low temperature phases. We will first give a short review of a refined BOS mixing model, which is used in lattice Monte-Carlo simulations. These simulations serve as input for the thermodynamic integration of free energies as function of size and composition. The resulting phase diagrams will be discussed for different particle sizes. We specifically address the question of how to interpet a two-phase regions in the phase diagram and explore the role of surface segregation. Finally, the kinetics of alloying processes is studied for free and supported particles by dynamic Monte-Carlo simulations.

O 60.6 Thu 11:30 MA 005

Doping of monoatomic Cu chains with single Co atoms — •Christophe Nacci, Jérôme Lagoute, and Stefan Fölsch — Paul Drude Institute for Solid-State Electronics, Hausvogteiplatz 5-7, 10117 Berlin, Germany

Close-packed Co-Cu chains (interatomic spacing 255 pm) of various length and composition were assembled from single Co and Cu atoms on Cu(111) by atom manipulation in a low-temperature scanning tunneling microscope [1]. Co atoms can be attached to monoatomic Cu chains to terminate the structure but also incorporated into the chain to occupy a predefined site. Local spectroscopy reveals significant electronic Co-Cu coupling leading to confined quantum states delocalized along the heteroatomic chain. The quantum state densities of composite Co-Cu chains are modified compared to those of pure Cu chains [2]. The modifications are well reproduced by a simple tight-binding analysis. Co-Cu chains provide an interesting model case in which the quantum state of an atomic-scale host structure can be tuned by the controlled incorporation of foreign atoms.

[1] J. Lagoute, C. Nacci, S. Fölsch, Phys. Rev. Lett. **98**, 146804 (2007)

[2] S. Fölsch, P. Hyldgaard, R. Koch, K. H. Ploog, Phys. Rev. Lett. **92**, 56803 (2004)

O 60.7 Thu 11:45 MA 005

Optical properties of supported core-shell and alloy silver/gold nanoparticles — •Frank Hubenthal and Frank Träger — Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

For many applications like surface enhanced Raman scattering in which the optical field enhancement associated with surface plasmon excitation is exploited, tunability of this collective resonance over a wide range is required. For this purpose we have prepared core-shell and alloy nanoparticles consisting of Ag and Au. The core-shell nanoparticles were made by subsequent deposition of Ag and Au atoms and vice versa on dielectric substrates followed by diffusion and nucleation. One of the most interesting among the numerous results is that the plasmon frequency can be tuned from 2.8 eV (442 nm) to 2.1 eV (590 nm) depending on the Au shell thickness. Subsequent annealing of the core-shell nanoparticles causes a shift of the resonance frequency to 2.6 eV. Theoretical modelling allows us to attribute this observation to the formation of alloy nanoparticles. Finally, we have measured the dephasing time T2 of the alloy nanoparticles by means of spectral hole burning. T2 amounts to 8.1 +/- 1.6 fs, in good agreement with the dephasing time T2 = 8.9 fs that is included in the dielectric function of the bulk.

O 60.8 Thu 12:00 MA 005

Tuning of the particle plasmon resonance in 2D and 3D polymer nanocomposites with bimetallic alloy particles prepared by vapor phase co-deposition — •Vladimir Zaporojtchenko, Venkata Sai Kiran Chakravadhanula, Haile Takele, Carolin Schulz, Thomas Strunskus, and Franz Faupel — Chair for Multicomponent Materials, Institute for Materials Science, Christian-Albrechts University at Kiel, Kaiserstr. 2, Kiel, Germany, 24143.

2D- and 3D- nanocomposite films consisting of bimetallic Ag-Cu or Ag-Au nanoparticles embedded in a nylon matrix were prepared by co-deposition of the components from three different evaporators in high vacuum. The microstructure of the nanocomposites and of the nanoparticles were investigated by TEM, XPS, XAFS, Electron Loss Spectroscopy and UV-Visible spectroscopy, with a focus on alloy formation, and the changes of the plasmon resonance bands. Shifts of the plasmon resonance of bimetallic alloy nanocomposites in a large spectral range (between 300 and 1000 nm) were observed by varying the ratio of the involved metals at a constant metal filling factor in the composites. The influence of substrate temperature on alloy formation in the core-shell nanoparticles was also studied. Shifting of the particle plasmon resonance either excited by light absorption or low energy electron scattering opens a new possibility to study the alloy formation in bimetallic nanoparticles.