O 60.1 Thu 9:30 MA 005
Invited Talk
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 Fe₁₋ₓCoₓ, alloy islands is highest for x = 0.5 and with Tₜₘ = 160 K two times higher than the one of pure Co (Tᵢ₀ = 90 K) or pure Fe islands (Tᵢ₀ = 80 K) of identical size and shape. This leads to an alloy contribution to the barrier for thermally induced magnetization reversal of E₂ₓ₃ ≈ 0.14 meV/atom. Co-core—Fe-shell islands reveal a steep increase of Tᵢ₀, 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 Tᵢ₀, similar to the one of pure Fe or Co. From this behavior we infer that the interface between Co and Fe contributes by Eᵢ₀ ≈ 0.9 meV/pair.

These values suggest 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.

O 60.2 Thu 10:00 MA 005
Invited Talk
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, diethylther 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.

O 60.3 Thu 10:30 MA 005
Invited Talk
Density functional studies of bimetallic nanosystems — Konstantin Neyman — ICREA, Dept. de Química Física & IQTUCB, 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 specie 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
Invited Talk
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 L¹₂ phase (lc). 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 modifications and enhanced ordering of L¹₂ 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 irradiation at low and elevated temperatures while taking into account defect production and sputtering yields as obtained from our MD-simulations.
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.