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Phase stability at small length scales: Segregation tendencies in nanoparticles of binary metallic alloys

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Abstract

Due to their nanoscopic sizes nanoparticles exhibit a surface-to-volume ratio which is significantly enhanced over that of their bulk counterparts. As a consequence, large fractions of the atoms “feel” the presence of these symmetry breaking surfaces or interfaces which go along with modifications of the local electron density, atomic coordination and bond lengths, to name a few. Concurrently, these alterations are to a large extent responsible for the widely appreciated novel properties of nanoparticles.

As a further consequence of the increased importance of surfaces at reduced dimensions, the surface (free) energies effectively compete with cohesive, strain, grain boundary and twinning energies and thus contribute significantly to the total energy balance of the particle. Hence, both the particle morphology and structure are increasingly affected by their surfaces. Specifically in alloy nanoparticles, differences in the surface (free) energies of the alloy constituents may promote the segregation of elements with low surface (free) energies toward these particle surfaces. As a consequence, compounds which are known to form homogeneous alloys in the bulk may exhibit the tendency to segregate at small length scales.

The talk will review segregation phenomena in alloy nanoparticles. Particular emphasis will be paid for the fingerprint-type surface-near lattice relaxation as determined through state-of-the-art aberration-corrected high resolution transmission electron microscopy (HRTEM). A particular focus will be laid on particles of binary metallic systems such as FePt, CuAu, FeNi, and AuFe, while elemental Au will serve as a reference material. The experimental HRTEM studies are corroborated by *in-situ* spectroscopic investigations such as local electron energy loss spectroscopy (EELS) and by molecular dynamics and Monte Carlo simulations.

Biography

Bernd Rellinghaus has earned his Ph.D. in Physics from the University of Duisburg, Germany. Awarded with a Research Stipend of the German Science Foundation, he then joined the IBM Almaden Research Center in San Jose, CA, USA. In 1997, he returned to Duisburg and moved to Dresden, Germany, in 2004, where he since then heads the Department for Metastable and Nanostructured Materials at the Leibniz Institute for Solid State and Materials Research (IFW Dresden). He is an expert in metallic materials, nanoparticles (particularly in nanomagnets) and in high resolution transmission electron microscopy. He has published about 100 papers in reputed journals.