MM 42: Nanostructured Materials III

Time: Thursday 14:00–15:45 Location: IFW A

MM 42.1 Thu 14:00 IFW A

Virtual diffraction of MD-simulated nanocrystalline Pd under compression — •Jürgen Markmann[1,2], Dmitriy Bachurin[3], Peter Gumbsch[3], and Jörg Weissmüller[1,2] — [1]Universität des Saarlandes, FR7.3 Technische Physik, 66123 Saarbrücken, Germany — [2]Forschungszentrum Karlsruhe in der Helmholtz-Gemeinschaft, Institut für Nanotechnologie, 76344 Eggenstein-Leopoldshafen, Germany — [3]Universität Karlsruhe, Institut für Zuverlässigkeit von Bauteilen und Systemen, 76131 Karlsruhe, Germany

Wide angle x-ray scattering (WAXS) is a widely used tool to characterise the microstructure of crystalline materials. During the last few years the means were developed to calculate x-ray spectra out of molecular dynamics simulation data and to use these spectra to analyse the MD structures. This approach has been validated to yield reliable results for well defined structures. Now, more realistic samples were investigated and analysed in-situ during a deformation by uniaxial compression. These samples consist of 100 randomly oriented palladium grains and were analysed for microstructural parameters like lattice constant, grain size, microstrain, and stacking fault density which can be evaluated out of the position and shape of the x-ray reflections. The most interesting finding is the increase of stacking fault density with the onset of plastic deformation. The stacking fault density reduces to zero when the structure is unloaded. This will be discussed togehter with the other microstructural parameters in terms of nucleation, dissolution, and movement of dislocations.

MM 42.2 Thu 14:15 IFW A

Segregation-induced near-surface lattice strain in CuAu nanoparticles — •Darius Pohl[1], Elias Mohn[1], Juri Barthel[2], Karsten Albe[3], Ludwig Schultz[1], and Bernd Rellinghaus[1] — [1]IFW Dresden, D-01171 Dresden, Germany — [2]FZ Jülich, D-52425 Jülich, Germany — [3]TU Darmstadt, D-64287 Darmstadt, Germany

For binary nanoparticles, experimental findings indicate the segregation of one alloy constituent towards the particle surface which leads to a surface-near relaxation of the lattice. Due to a difference in the surface free energies between copper and gold, a gold segregation for nanoparticles is expected. In the case of CuAu nanoparticles, Au segregation towards the surface is suggested to lead to a lattice expansion. Through aberration-corrected HRTEM imaging with minimum delocalisation is achieved, and the position of individual atom columns can be determined with unrivalled precision.

Molecular dynamic (MD) simulations of CuAu nanoparticles are conducted under the constraint that the particle surface is terminated with either Cu or Au. A comparison between HRTEM contrast simulations of the simulated structures and experimental HRTEM images then allows to distinguish between the different possible scenarios. It is hereby proven that single crystal CuAu nanoparticles with a mean diameter of 3 nm exhibit a lattice relaxation due to a segregation of Gold atoms. This finding is in agreement with previous results obtained for multiply twinned FePt nanoparticles and thus corroborates that the surface-near expansion of the lattice is due to a segregation rather than to internal stress within the particle structure itself.

MM 42.3 Thu 14:30 IFW A

Size-dependence melting transformation of nanoparticles confined in an Al-rich glass — •Nancy Boucharat[1], Harald Rösner[2], and Gerhard Wilde[2] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Karlsruhe — [2]Universität Münster, Institut für Materialphysik, Münster

A common way to study the size dependence of the melting transformation is given by incorporating nanoparticles within a matrix. This configuration implies additional contributions related to the nature of the interfaces between the particles and the host matrix which strongly affect the melting process. Thus, the incorporation of nanoparticles within a glassy matrix opens a new angle to revise the size-dependence of melting by limiting the constraints imposed on the particles by the presence of a crystalline matrix with anisotropic lattice mismatch. Here, AlYFe glasses containing immiscible Pb or In additions have been synthesized via rapid solidification. As expected for liquid-liquid phase separation, the Pb-containing samples consist of spherical Pb inclusions homogeneously dispersed within the matrix. In contrast, the In-containing samples show non-crystalline In-enriched regions. Applying a subsequent low-temperature treatment involves the crystallization of spherical particles with sizes smaller than 5 nm, which melt at extremely low temperatures compared to the bulk material. In this context, the melting behavior is discussed with respect to the size dependence and to the energetic contributions from the particle/matrix interfaces.

MM 42.4 Thu 14:45 IFW A

Gold nanoparticles under synchrotron X-rays — •Chang-Hai Wang[1], Chi-Jen Liu[2], Tzu-En Hua[2], Chia-Chi Chien[2], Wei-Hua Leng[2], Shin-Tai Chen[2], Cheng-Liang Wang[2], and Yeu-Kuang Hwu[2] — [1]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55099 Mainz — [2]Institute of Physics, Academia Sinica, Taipei, 11529 Taiwan

Gold particles with length scale less than 100 nm develop unique physical properties and biocompatible features that render extensive applications in nanotechnology. To materialize the functionalities, gold nanoparticles with controlled size, favorable surface properties and size distribution would be a pre-requisite. This work describes a new room-temperature synchrotron X-ray irradiation method to prepare reductant- and stabilizer-free colloidal gold solutions. Typical characterization tools include TEM, UV-VIS, FTIR, XRD and ICP-OES. The influence of processing parameters such as the pH value, exposure time, ionic strength and radical scavenger on the structure of gold nanoparticles was investigated. The mechanisms underlying the X-ray-triggered reduction of gold ions and the formation of gold clusters are discussed in detail. An interesting morphological evolution as a function of exposure time, from cross-linked network-like structure to individual particles, has been discovered. This approach could be easily extended to the preparation of polymer-modified colloidal gold by simply adding the polymer species to the precursor solutions. As an implication for nanotechnology, the interactions between gold nanoparticles and cells are also studied and reported.

MM 42.5 Thu 15:00 IFW A

Temperature dependent vibrational fingerprints of gold nano clusters: a DFT study — •Luca Ghiringhelli and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

The study of gold nanoclusters is a flourishing topic, due to its importance for catalysis and the presence of unexpected phenomena (e.g. chirality). Here, we apply the recently developed all-electron ab-initio code "FHI-aims" for the density functional (DFT) study of the relative energies and vibrational properties of known isomers of small Au_n ($n \leq 10$) clusters. In particular, besides the calculations of the traditional harmonic frequencies, we focus on the less common evaluation of the (temperature dependent) vibrational spectrum, via Fourier transform of the velocity autocorrelation function, where the velocities come from DFT based Molecular Dynamics trajectories at given temperatures. We underline differences between harmonic and an-harmonic spectra at different temperatures and compare with available experimental data.

MM 42.6 Thu 15:15 IFW A

Delocalization mechanisms of excess free-volume in nanoglasses — •Daniel Sopu[1], Karsten Albe[1], Yvonne Ritter[1], and Herbert Gleiter[2] — [1]Institut für Materialwissenschaft, TU Darmstadt, Petersenstr. 23, D-64287 Darmstadt, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, P.O. Box 3640, D-76021 Karlsruhe, Germany

Molecular dynamics simulations are presented which provide a detailed picture of the structure of nanoglasses, a class of material which can be synthesized by consolidating nanometer-sized glassy particles. Our results provide evidence the existence of glass-glass interfaces between the consolidated particles. These interfaces are characterized by an excess free volume. By comparing simulations for covalently bonded Ge nanoglass and metallic CuZr nanoglass, we find that the delocalization of this free volume is driven by homogeneous plastic flow and by thermally activated diffusion. These results suggest that the overall density, microstructure and atomic structure of nanoglasses can be adjusted by the initial particle size and chemical composition as well as by the annealing conditions.

MM 42.7 Thu 15:30 IFW A

Mechanical alloying of Fe-Cu powders: elaborating the microstructure at various scales — •Catharina Wille[1], Taláat Al-Kassab[1,2], Pyuck-Pa Choi[3], and Reiner Kirchheim[1] — [1]Institut für Materialphysik, Universität Göttingen, Germany — [2]Material Science and Engineering, King Abdullah University of Science and Technology (KAUST), effective 15 April 2009 — [3]Korea Institute of Science and Technology, Nano-Materials Research Center

In this contribution, the process of mechanical alloying has been studied for both sides of the binary Fe-Cu system. Ranging from light-optical microscopy on the mm-scale to atom probe tomography (APT) on the Ångstrøm-scale, the morphology could be observed on several orders of magnitude. Since a ductile element (Cu, fcc) and a brittle one (Fe, bcc) were combined, striking differences in morphology were expected and found on all length-scales, depending on the mixing ratio. Results on powders with low concentrations of the respective minority component will be presented and discussed.

Regarding the widespread application and accessibility, Fe-Cu acts as an ideal binary model alloy to elaborate the enforced non-equilibrium enhanced solubility being immiscible and characterised by a large positive heat of mixing. Chemical identification on the Ångstrøm-scale was granted by APT. Thus, not only the atomic mixing of Fe and Cu could be evaluated, but also the distribution of impurities, mostly stemming from the fabrication procedure.

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