# MM 53: Nanostructured Materials IV

Time: Thursday 14:00–15:00 Location: H16

MM 53.1 Thu 14:00 H16

**Strain in the nanograin** — •Harald Rösner and Gerhard Wilde — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster, Germany

Strain in an individual deformation-twinned nanocrystalline Pd grain of about 24 nm size was mapped. The in-plane components of the strain tensor were calculated and charted using geometric phase analysis based on an individual high-resolution transmission electron microscopy image. Considerable shear strain was accumulated along the twin boundaries. The twins and matrix were significantly distorted relative to each other (rotated by about 3° on average) and showed a strong gradient across the grain running parallel to the twin lamellae. An estimate of the strain energy stored in the Pd grain yielded a value of E = 6.495 J/g. Based on the strain distribution observed, a temporal deformation scenario is discussed.

MM 53.2 Thu 14:15 H16

**Melting behaviour of embedded Pb nanoparticles in an Al (Ga) matrix** — •Anna Moros, Harald Rösner, and Gerhard Wilde — Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Melting is one of the most important phase transformation in nature, but its underlying mechanism is still not completely understood. It is well known, that decreasing particle sizes lead to a change of the bulk properties of a material, as for instance a shift of the melting point. Current investigations on the melting behaviour of Pb nanoparticles embedded in an Al matrix are presented. In contrary to the prediction of many models for size-dependent melting, faceted and truncated cuboctahedric Pb nanoparticles with a cube-on-cube orientation relationship to the matrix start to melt 10 - 30 K above the melting point of the bulk material, indicating a more complex dependence of the melting temperature with respect to the particle-matrix interfaces. Here, the melting temperature of the particles was determined by means of differential scanning calorimetry. The size distribution of Pb inclusions in the samples was obtained from TEM images. However, it was observed that the addition of Gallium selectively into the Al matrix led to a significant shift of the melting temperature of the Pb nanoparticles. The experimental results are presented and discussed.

MM 53.3 Thu 14:30 H16

**Finite Size Effects in Oxide Nanoparticles** — •Manuel Diehm, Peter Agoston, and Karsten Albe — Technische Universität Darmstadt, Institut für Materialwissenschaft, Petersenstr. 23, 64287 Darmstadt

Nanoparticles of several oxide materials with different structures and morphologies are investigated by molecular statics simulations in order to study the implications of finite size effects. Interatomic interaction was described by Coulomb/Buckingham pair-potentials and special attention was given to the role of missing long-ranged Coulomb interactions and related structural relaxations. It is discussed under what conditions volume and surface contributions to the lattice energy of ionic nanoparticles become extensive quantities. Further, it is examined how the presence of point defects affects the lattice energy and the range of resulting disturbances in the ideal Coulomb potential at surrounding lattice sites.

MM 53.4 Thu 14:45 H16

**Simulation of the gyroid phase in copolymer systems** — •Alexei Karatchentsev[1], Wolfgang Dieterich[2], Philipp Maass[3], and Jens-Uwe Sommer[1] — [1]Leibniz-Institut für Polymerforschung, 01069 Dresden, Germany — [2]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [3]Fachbereich Physik, Universität Osnabrück, 49069 Osnabrück, Germany

We employ a coarse-grained model to study the formation of periodic continuous mesostructures in diblock and triblock copolymer melts. Within this model, the blocks of the copolymer molecule are mapped onto soft spheres with fluctuating radii of gyration and the distance between the centers of the spheres [1]. The probability distribution functions for these quantities as well as the monomer number densities of the blocks are derived from the Gaussian chain model. The kinetics of the mesophase segregation is driven by a Monte-Carlo algorithm. First we explore in detail the gyroid phase observed in the diblock copolymer system and discuss its stability. Then we study the system of linear triblock copolymers and show how such system can possibly increase the region of stability of the gyroid phase.

[1] F. Eurich, A. Karatchentsev, J. Baschnagel, W. Dieterich, and P. Maass J. Chem. Phys. 127, 134905 (2007)