MM 34: Nanomaterials

Grain Boundaries and Interfaces

Time: Wednesday 11:45–12:45 Location: H 0106

MM 34.1 Wed 11:45 H 0106

Equilibrium nanoparticle shapes for any size from atomistic simulations — •Magnus Rahm and Paul Erhart — Department of Physics, Chalmers University of Technology, Gothenburg, Sweden

In the pursuit of complete control over morphology in nanoparticle synthesis, knowledge of the thermodynamic equilibrium shapes is a key ingredient. While the classical Wulff construction provides a solution in the continuum limit, the small particle regime has been studied using global minimum energy search method reaching particle diameters of roughly 1 or 2 nm. The experimentally important intermediate size regime, however, has largely remained elusive. Here, we present an algorithm, based on atomistic simulations in a constrained thermodynamic ensemble, that efficiently predicts equilibrium shapes for any number of atoms in the range from a few tens to 10,000, corresponding to diameters between approximately 1 and 7 nm. We apply the algorithm to Cu, Ag, Au and Pd and reveal an energy landscape that is more intricate than previously suggested. In particular, we demonstrate that, as a result, the transition from icosahedral particles to decahedral and further into FCC particles occurs very gradually. One must thus expect more than one shape in thermodynamic equilibrium and not only for for kinetic reasons.

MM 34.2 Wed 12:00 H 0106

A Live Broadcast From Within Deforming Nanocrystalline PdAu Aggregates — •Michael Johannes Deckarm[1], Andreas Leibner[1], Marta Majkut[2], Vadim Dyadkin[2], and Rainer Birringer[1] — [1]Saarland University, D-66123 Saarbrücken — [2]ESRF, F-38043 Grenoble Cedex 9

Scaling the grain size of PdAu down to the low end of the nano scale (≈ 10nm) entails a dramatic change in mechanical properties. In a recent study, Grewer et al. [1] examined the deformation of nanocrystalline PdAu in an in-situ experiment using a combination of optical strain and synchrotron-based X-ray diffraction measurement. The central result was a quantitative estimate of the contributions of various processes to the deformation. In continuation of this work, we explored the effects of different strain rates and stress states, respectively, by a series of experiments at beamline ID11 at the ESRF. Scattering data with high temporal resolution spanning the entire deformation provide us with a broadcast of the evolving stress state. Specifically, we discuss a whole powder pattern modelling approach to extract structural information from our scattering data [2], to then reconstruct average stress and strain states of differently oriented grains as well as the signature of the elastic anisotropy of PdAu crystallites and its relation to the stresses or strains arising from the compatibility constraints in nanocrystalline PdAu aggregate.

[1] M. Grewer et al., Mechanics of Materials, 114, 2017, 254-267 [2] Scardi, P; Leoni, M., Acta crystallographica. Section A, Foundations of crystallography., 57., 2001, 604-613.

MM 34.3 Wed 12:15 H 0106

Evaluation of tension-compression asymmetry in nanocrystalline PdAu using a Drucker-Prager type constitutive model — •Andreas Leibner[1], Michael Deckarm[1], Hasan Raza Syed[2], Benjamin Klusemann[2], and Rainer Birringer[1] — [1]Experimentalphysik, Universität des Saarlandes — [2]Institut für Produkt- und Prozessinnovation, Leuphana Universität Lüneburg

There is ample evidence that the deformation behavior in nanocrystalline materials differs significantly from their coarse grained counterpart [1]. NC PdAu alloys at the low end of the nanoscale (≈ 10nm), where plasticity is predominantly mediated by grain boundaries [2], exhibit a distinct tension*compression asymmetry, which is unusual for fcc metals.

We performed deformation experiments utilizing a specific geometry. Tuning this geometry allows one to tailor the state of stress, in terms of compression to shear ratio, in the gauge section of the specimen. In order to evaluate the general deformation behavior of NC PdAu we employed FEM simulations and used a customized Drucker-Prager type constitutive material model.

In particular, we studied four different specimen geometries and varied the strain rate over five orders of magnitude down to 10^{-5}. As a result, we find an intriguing variation of deformation and failure behavior. Nevertheless, we tried to explore whether or not a single material law is capable of capturing the stress strain evolutions.

[1] E.N. Hahn and M.A. Meyers, Mat. Sci. Eng. A, 646 (2015) 101-134 [2] M. Grewer et al., Mechanics of Materials, 114 (2017) 254-267

MM 34.4 Wed 12:30 H 0106

Influence of local grain boundary structure on electronic transport in polycrystalline graphene — •Delwin Perera, Jochen Rohrer, and Karsten Albe — Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

Graphene is a promising material for microelectronics and sensor technology due to its high charge carrier mobility, high strength and optical transparency. Recently, it was found that nanocrystalline graphene is piezoresistive which makes it suitable for strain sensing [1]. Theoretical studies attribute this piezoresistivity to grain boundaries, which can induce transport gaps. The size of the transport gap is believed to depend only on the misorientation of adjacent grains [2].

Here, we investigate the effect of the local grain boundary structure on the electron transport properties of graphene. We use density functional theory together with the non-equilibrium Green's functions formalism to calculate transmission functions and current-voltage curves within the ballistic approximation [3]. Our results show that the size of the transport gap is indeed not affected by local structural changes. However, the details of the transmission function are sensitive to the local grain boundary structure. Therefore, the current-voltage characteristics depend not only on the misorientation.

[1] Riaz *et al.*, Nanotechnology **26**, 325202 (2015)
[2] Kumar *et al.*, Nano Lett. **12**, 1362 (2012)
[3] Brandbyge *et al.*, Phys. Rev. B **65**, 165401 (2002)