MM 33: Topical Session Theory meets Experiment II - Nanocomposites and Microstructure

Time: Wednesday 11:30–13:00 Location: TC 006

Topical Talk MM 33.1 Wed 11:30 TC 006

Correction of spherical and chromatic aberration: towards the ultimate performance in transmission electron microscopy — •Joachim Mayer — Central Facility for Electron Microscopy, RWTH Aachen University, 52074 Aachen and Ernst Ruska-Centre, Forschungszentrum Jülich, 52425 Jülich

The introduction of aberration correctors has revolutionized the development of TEM and STEM instrumentation. Only shortly after the development and installation of the first TEM with a corrector for the spherical aberration [1], commercial instruments with aberration correctors are now offered by all major manufacturers. In order to provide a platform for these novel developments and based on the experience with the first aberration corrected TEM [2], Research Centre Juelich and RWTH Aachen University have jointly founded the Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons (ER-C). With the recent installation of PICO, the second high resolution TEM in the world which is equipped with a corrector for the chromatic aberration, a broad range of new methods is now available. Research at the Ernst Ruska-Centre focuses on the development of new quantitative methods in TEM and on their application in materials science and solid state physics [3]. The most important fields of application are nanoelectronics and nanomaterials for energy-related systems. [1] M. Haider, H. Rose, S. Uhlemann, E. Schwan, B. Kabius, and K. Urban, Nature 392 (1998) 768. [2] C.L. Jia, M. Lentzen, and K. Urban, Science 299 (2003) 870. [3] C. L. Jia, S. B. Mi, K. Urban, I. Vrejoiu, M. Alexe, D. Hesse, Nat. Mater. 7 (2008) 57.

MM 33.2 Wed 12:00 TC 006

Atomic modeling of asymmetric tilt grain boundaries in Al_2O_3 — •Haksung Lee[1], Paul Tangney[2], Matthew Foulkes[1], and Michael Finnis[1,2] — [1]Department of Physics, Imperial College London, Exhibition Road, London SW7 2AZ, UK — [2]Department of Materials, Imperial College London, Exhibition Road, London SW7 2AZ, UK

The atomic level characterization of grain boundaries is a fundamental subject in materials science and condensed matter physics because grain boundaries drastically affect the physical properties of polycrystalline materials. Thus the atom arrangement, termination plane, chemical composition, and electronic structure of grain boundaries, and in particular symmetric tilt grain boundaries, have been extensively investigated both experimentally and theoretically. In contrast, there are few studies of asymmetric tilt grain boundaries, despite being more prevalent, and therefore more significant to the material properties, than symmetric tilt grain boundaries.

In this presentation we introduce two symmetric and two asymmetric tilt [0001] $\Sigma 7$ grain boundaries in Al_2O_3 through geometrical considerations. To find the stable grain boundary core structure, many configurations for each boundary were calculated using interatomic potentials. Interestingly, the grain boundary energies of the two asymmetric tilt grain boundaries are very similar to those of the symmetric tilt grain boundaries with the same Coincidence Site Lattice. We analyse the structures that emerge and compare the results with existing experimental data.

MM 33.3 Wed 12:15 TC 006

Deformation mechanisms of twinned Au-nanoparticles under compression: Experiments and Simulation — •Andreas Kelling[1], Cynthia A. Volkert[1], Wolfram Nöhring[2], and Erik Bitzek[2] — [1]Institut für Materialphysik, Universität Göttingen, D-37077 Göttingen — [2]Lehrstuhl WWI: Allgemeine Werkstoffeigenschaften, Universität Erlangen-Nürnberg, D-91058 Erlangen

The plastic deformation of nanoscale metallic specimens has recently attracted a lot of interest due to the reported changes of deformation mechanisms with reduced size. Here, we present compression experiments and atomistic simulations of gold nanoparticles to study dislocation processes and -storage in nanosized volumes. The particles are 80 and 250 nm in size and have faceted self-similar triangular shapes. They contain a twin boundary parallel to their upper and lower (111) surfaces. The particles are compressed along the [111] axis using a nanoindenter with a flat punch tip up to a strain of 50%. No dislocations were observed before deformation. Post-mortem TEM-analysis of both particle sizes reveals the storage of full dislocations. No difference in dislocation type is observed for the two different particle sizes. Molecular Dynamics simulations of Au particles with the same shapes were performed using different types of indenters and boundary conditions. The processes of dislocation nucleation, reactions, cross-slip and interactions with the twin boundary are studied in detail and analyzed in terms of the overall stress state. Comparison with the experimental microstructure allows us to draw conclusions about the dominant dislocation processes during the deformation of the particles.

MM 33.4 Wed 12:30 TC 006

Properties of fivefold twinned nanowires derived from microstructural constraints and anisotropic elasticity — •Florian Niekiel[1], Erdmann Spiecker[1], and Erik Bitzek[2] — [1]Center for Nanoanalysis and Electron Microscopy (CENEM), Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Institute I: General Materials Properties, Department of Material Science and Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg

Fivefold twinned metallic nanowires of fcc crystal structure have lately attracted a lot of attention because of their interesting properties and potential applications. Such nanowires consist of five segments, which are joined by {111}-twin boundaries, sharing a common crystal direction along the wire axis. The angular misfit of 7.35° resulting from joining the five wedge shaped segments necessitates the existence of a positive partial wedge disclination at the quintuple line present in the center of the nanowire. This peculiar microstructural constraint gives rise to significantly different properties of fivefold twinned nanowires in comparison to their single crystalline counterparts.

Here atomistic simulations and experimental diffraction measurements are combined to study the stress and strain state in fivefold twinned nanowires. Based on the findings a theoretical framework accounting for anisotropic elasticity is developed to quantitatively predict the mechanical properties of such nanowires as function of the used material. In this way the model helps not only to understand the properties of fivefold twinned structures but also to design their properties for future applications.

MM 33.5 Wed 12:45 TC 006

Mechanical and magnetic properties of Mn–Pt compounds and nanocomposites — •Tomáš Káňa[1] and Mojmír Šob[2,3,1] — [1]Institute of Physics of Materials, Brno, Czech Republic — [2]Central European Institute of Technology, CEITEC MU, Brno, Czech Republic — [3]Faculty of Science, Masaryk University, Brno, Czech Republic

An analysis of mechanical and magnetic properties of Mn–Pt compounds and nanocomposites is provided using DFT calculations. Adding manganese to platinum matrix reduces the bulk modulus and enhances the Young moduli E_{100}, E_{111} as well as shear moduli $(c_{11} - c_{12})/2$ and c_{44}. With increasing Mn content, the theoretical tensile strength is also enhanced and the corresponding maximum deformation is reduced. On the whole, manganese addition makes the Mn–Pt compounds softer, but increases their resistance to shape deformation. Many of these compounds may be considered as natural linear nanocomposites. We studied the magnetic configurations of recently found $MnPt_7$ ordered structure and predict an antiferromagnetic state with spins altering along the [100] direction to be the ground state of this compound. We further studied Mn–Pt nanocomposites with the composition of $MnPt_{15}$. Here an antiferromagnetic structure with spins altering along the [100] direction is the ground state of $MnPt_{15}$ nanocomposite. The alternative ferromagnetic configurations of different $MnPt_{15}$ nanocomposites exhibit the screening of magnetic moments of Mn atoms by flipping the moments induced on Pt atoms into the opposite direction. This indicates that the Mn spins can be coupled through the Pt atoms.