MM 8: Topical session (Symposium EPS and MM): Mechanical Properties at Small Scales

Plasticity: Modelling

Time: Monday 11:45–13:15 Location: TC 006

Topical Talk MM 8.1 Mon 11:45 TC 006

Deformation twinning in nanostructured metallic systems: molecular dynamics study — •Sandrine Brochard, Romuald Béjaud, and Julien Durinck — Institut PPRIME - Poitiers-Futuroscope - France

At the nanoscale, mechanical twinning seems to be promoted, as shown e.g. in thin films or nanocrystalline materials. This trend is also true for metallic nanolayered composites obtained by severe plastic deformation processes. In such materials, interfaces may act as partial dislocation and deformation twin sources, and the interfaces structure is expected to have a key role in twin propagation and thickening.

In this study, we investigate how different interface types influence the main stages of mechanical twinning. Because of the small length and times scales at which the elementary plasticity mechanisms involved occur, molecular dynamics simulations prove to be relevant and efficient tools.

Heterophase interfaces in a bimetallic Cu/Ag system, as well as a coherent twin boundary (CTB), are examined in a similar thin film geometry. A reference case with no planar defect inside the thin film is also considered. For both systems with "heterotwin" heterophase interface and CTB, the deformation twins are smaller, consistent with the low permeability of these interfaces to dislocations. But twins are more numerous, which is correlated to Lomer dislocation nucleation. For the Cu/Ag film with a "cube on cube" type interface, our simulations reveal the specific role of the misfit dislocation mesh in twin extension from the interface.

MM 8.2 Mon 12:15 TC 006

Multi-scale modeling of dislocations behavior in molybdenum — •Sergei Starikov[1,2] and Vasily Tseplyaev[1] — [1]Joint Institute for High Temperatures, Moscow, Russia — [2]ICAMS, Ruhr-Universität Bochum, Germany

Various types of computer simulation were performed for study of dislocations behavior in molybdenum. Molybdenum is typical body-centered cubic metal and such study allows to understand basic properties of plasticity in bcc metals. Multi-scale approach consists from combination of different methods which one calculates properties at various scales. We used three different models: development of an interatomic potential on the basis of ab-initio calculations; molecular dynamics simulations; dislocation dynamics. Such multi-scale approach allows us to investigate the dislocation properties in molybdenum and compare the simulation results with the available experimental data. Particular attention is given to the link between models at various scales and calculations of macroscopic features (like stress-strain curve).

MM 8.3 Mon 12:30 TC 006

Atomistic simulations of the mechanical behavior of semiconductor and metallic nanoparticles — Dimitrios Kilymis[1], Sélim Bel Haj Salah[1], Céline Gérard[1], Jonathan Amodeo[2], and •Laurent Pizzagalli[1] — [1]Institut Pprime, CNRS UPR 3346, Université de Poitiers, Poitiers, 86962, France — [2]MATEIS, CNRS UMR 5510, INSA-Lyon Université 1, Villeurbanne, 69621, France

We present the results of molecular dynamics simulations of the mechanical properties of semiconductor and metallic nanoparticles. The aim of the study is to investigate the first stages of plasticity during uniaxial compression while focusing on the influence of the shape (spherical, or facetted, or cubic geometries) and size (from 10 to 50 nm). The nanoparticles are deformed at a constant velocity using flat punch indenters, along different orientations in most of cases. We fully characterize the onset of plasticity, both in terms of yield point and of mechanisms, and examine how those depend on the size and the shape of the nanoparticle. The influence of temperature is also considered. In the case of semiconductor nanoparticles, original plasticity mechanisms are identified, including V-shaped dislocations and an hexagonal phase transition of limited extent. Conversely, for metallic systems, the first plasticity mechanisms are similar to the ones usually activated in bulk. In both cases, it is found that both size and shape effects are significant for the investigated systems.

MM 8.4 Mon 12:45 TC 006

Effect of hard amorphous shell on gold nanowire during mechanical cycling — •Maxime Guillotte, Laurent Pizzagalli, and Julien Godet — Pprime Institute, CNRS, University of Poitiers - France

In order to evaluate the role of a hard amorphous silicon (a-Si) shell on the deformation of a soft crystalline gold core, we have investigated the mechanical properties under tensile and compressive cycling of the Au@a-Si core-shell nanowire (NW) by molecular dynamics simulations. We used an existing parametrization of the MEAM potential that has been optimized to better reproduce the mechanical properties of gold and silicon as well as the Au-Si interactions. The comparison of the mechanical tests performed on pristine Au NW and Au@a-Si core-shell NW reveals that the hard amorphous shell is able to confine the plasticity inside de core. In consequence, the localized plasticity and the expansion of nano-twin are reduced. The confinement of the dislocations in the core also leads to a homogeneous plastic deformation of the core-shell nanowire at almost constant flow stress equal to the yield stress up to a strain of 50%. This behavior is characteristic of an elastic/perfect-plastic mechanical regime. During the cycling tests, it also seems that the hard amorphous shell is is at the origin of the recovery of the FCC core.

MM 8.5 Mon 13:00 TC 006

Plasticity of silicon at small scale and low temperature: an experimental and numerical study — •Michael Texier[1], Amina Merabet[1], Firas Abed El Nabi[2], Christophe Tromas[2], Sandrine Brochard[2], Laurent Pizzagalli[2], Ludovic Thilly[2], Jacques Rabier[2], Anne Talneau[3], Olivier Thomas[1], and Julien Godet[2] — [1]IM2NP, UMR7334 CNRS - Univ. Aix-Marseille, Marseille, FR — [2]Pprime, UPR3346 CNRS - Univ. Poitiers, Futuroscope, FR — [3]C2N, Univ. Paris Sud, Orsay, FR

Mechanical properties of silicon have been widely studied in the last decades, but recent studies evidenced that silicon nano-objects behave differently than bulk materials when submitted to mechanical stress. Indeed, for dimensions below a few hundreds of nanometres, a brittle-to-ductile transition (BDT) occurs at room temperature and its origin remains undetermined. Although essential for the Si-based nanotechnologies, the understanding of the microscopic mechanisms responsible for this behavioural change requires to compare results obtained from well-controlled deformation experiments at smallest scales with realistic numerical simulations. In this work, both experimental and numerical nano-compression tests were carried out on similar Si nanopillars. Results obtained from simulations and HRTEM analyses of the deformed specimen disrupt the established description of undissociated-dislocations-mediated plasticity of silicon at low temperatures. This study allows deeply reinterpreting the experimental data recently reported in the literature, and highlights the intricate relationship between BDT, dislocation interactions, and size effect.