MM 19: Mechanical Properties I

Time: Tuesday 10:15–11:45 Location: H52

MM 19.1 Tue 10:15 H52

FUNDAMENTAL NANOMECHANIC INVESTIGATIONS USING COMBINATORIAL DEPOSITION TECHNIQUES — •Rachel Schoeppner, Laszlo Petho, and Johann Michler — Empa, Materials Science and Technology, Thun, Switzerland

We've designed a unique deposition system combining magnetron sputtering, e-beam evaporation, nanoparticle deposition and atomic layer deposition (ALD). An integrated shutter controller allows for creating thickness gradients of two or three different materials, which can then be annealed to create a combinatorial materials library with compositional gradients over almost the complete spectrum. Initial studies of the system capability have focused on proof-of-concept trilayer systems consisting of Al2O3 and TiO2 ALD layers sandwiched between thicker Cu layers deposited by sputtering. Physical and mechanical characterisation of these trilayers, including micropillar compression, has demonstrated good interfacial adhesion and that even just a single ALD layer, only nanometers thick, can provide significant hardening to Cu thin films. Combinatorial libraries of ternary AlCuAu and AuAgPt alloy systems have been used in an adhesion study to examine the effect of composition on interfacial adhesion, between the film and a 500 nm thick layer of Al2O3 deposited using ALD. Finally, Cu films were reinforced via co-deposition of W nanopartices. The microstructure, particle size and density were characterized using transmission electron microscopy and initial nanoindentation investigations were conducted to determine how nanoparticle inclusion affects the hardness and modulus of the films.

MM 19.2 Tue 10:30 H52

Flaw sensitivity of nanowires — •Christian Brandl — Institute for Applied Materials, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany

With decreasing dimensions of the metals, the strength is increasing with decreasing dimensions can approach the theoretical strength limit - down to a regime, where the strength is theoretically predicted to be flaw insensitive.

Using atomic simulation, we investigate the effect of predefined flaws, i.e. notches, in intrinsic brittle Si nanowires and intrinsic ductile Au nanowires. The flaw size and wire diameter dependent strength and ductility in the molecular dynamics (MD) simulations show the existence of the flaw insensitive size regime. The defect evolution, flow stresses and the strain hardening in the MD simulations of Au nanowires is compared to experimental studies, where gold nanowires were structured by He-ion beams with sub-50 nm diameter well-defined holes. The experimental microstructure after deformation - as seen by (high-resolution) transmission electron microscopy - suggests the formation of a nano-grained substructure at the failure location, which is also consistently observed in our MD simulation.

The striking similarities between MD simulations and the experimental data are critically discussed and explained by strain hardening in a strength regime of theoretical shear strength in Au. More generally, the implications of strain rate dependence and temperature dependence of the flow stresses are discussed for nanowires in the size regime of flaw insensitivity.

MM 19.3 Tue 10:45 H52

Metamaterials using buckling instabilities for reusable energy absorbers — •Tobias Frenzel[1], Claudio Findeisen[2,3], Muamer Kadic[1], Peter Gumbsch[2,3,4], and Martin Wegener[1,4] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — [2]Institute for Applied Materials, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — [3]Fraunhofer Institute for Mechanics of Materials IWM, 79108 Freiburg, Germany — [4]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany

Commonly, structures and materials for mechanical energy absorption exploit either viscoelasticity or plasticity. While viscoelasticity leads to a reusable, yet time-dependent behavior, plasticity is not influenced by the timescale, yet the structural deformation is irreversible. In this work, we introduce a new class of artificial material, which exploits elastic buckling in a uniaxial micro-lattice as a mechanism for energy absorption. Most importantly the energy is not dissipated by local effects, e.g., within one unit cell, but by the coupling of N effectively nonlinear springs in series. By tailoring the buckling elements, either a hysteretic, yet repeatable, or a multi-stable behavior enabling for programmability can be achieved. Furthermore, the shape of the stress-strain curves can be tailored, which allows for control over peak forces. Experiments performed on polymer micro-structures made by direct laser writing scaled to aluminum show specific energy absorption comparable to state-of-the-art aluminum-foams.

MM 19.4 Tue 11:00 H52

Scaling laws of nanoporous gold under uniaxial compression: Effects of structural disorder on the solid fraction, elastic Poisson's ratio, Young's modulus and yield strength — •Benedikt Roschning[1] and Norbert Huber[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology — [2]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht

Recent investigations on the mechanical behavior of nanoporous gold [1,2,3] led to inconsistencies to previous results (summarized in [4]) indicating that the material's coupling behavior between the solid phase and the macroscopic mechanical response is still not fully clarified. We investigated the relationship between the structural disorder and the macroscopic mechanical behavior of nanoporous gold under uniaxial compression, using the finite element method. Scaling equations for the elastic Poisson's ratio, the Young's modulus and the yield strength were determined as functions of the structural disorder and the solid fraction. The model was applied to identify the elastic-plastic material behavior of the solid gold phase. Based on this approach, a systematic study of the size effect on the yield strength was performed and the results were compared to experimental data provided in literature. An excellent agreement with recently published results for samples of nanoporous gold with varying ligament size was found. [1] Huber, N., et al. 2014. Acta Materialia 67, 252-265. [2] Jin, H.-J., et al., 2009. Acta Materialia 57, 2665-2672. [3] Wang, K., et al., 2015. NPG Asia Mater 7, e187. [4] Weissmüller J., et al., 2009. MRS Bulletin 34, 577-586.

MM 19.5 Tue 11:15 H52

Stacking fault energetics of α- and γ-cerium investigated with ab initio calculations — •Andreas Östlin[1], Igor di Marco[2], Inka Locht[2], Jason Lashley[2,3], and Levente Vitos[1,2,4] — [1]Applied Materials Physics, Department of Materials Science and Engineering, KTH Royal Institute of Technology, Stockholm SE-100 44, Sweden — [2]Department of Physics and Materials Science, Uppsala University, P.O. Box 516, SE-75120 Uppsala, Sweden — [3]Los Alamos National Laboratory, P.O. Box 1663 Bikini Atoll Road, Los Alamos, New Mexico, USA — [4]Research Institute for Solid State Physics and Optics, Wigner Research Center for Physics, Budapest H-1525, P.O. Box 49, Hungary

At ambient pressure the element cerium shows a metastable double hexagonal close-packed β-phase that is positioned between two cubic phases, γ and α. We have computed stacking fault formation energies of the cubic phases of cerium using an axial interaction model. Total energies were calculated by density functional theory (DFT) and by dynamical mean field theory (DMFT) merged with density functional theory (DMFT+DFT). It is found that there is a large difference in the stacking fault energies between the α and γ-phase. The β-phase energy is nearly degenerate with the γ-phase, consistent with previous third law calorimetry results, and dislocation dynamics explain the pressure and temperature hysteretic effects. The β-phase can be seen as a dislocation reservoir that appears to be necessary to accommodate the large strains generated during the α-γ transition.

15 min. coffee break