MM 6: Mechanical Properties II

Time: Monday 11:30–12:45 Location: H 0106

MM 6.1 Mon 11:30 H 0106

Dislocation microstructure evolution and size effect during torsion of thin single crystalline metallic wires: a discrete dislocation dynamics approach — Jochen Senger and •Daniel Weygand — Karlsruhe Institute of Technology, IAM, Karlsruhe, Germany

The ground breaking investigations of Fleck [1] on the size dependence observed by applying torsion boundary constraints have – to the authors knowledge – not been addresses by 3D discrete dislocation dynamics (3DDD). Under torsion, the trend smaller is stronger has been found. This observation has been a motivation for strain gradients approaches. Despite this a detailed knowledge on the dislocation microstructure, characteristic for torsion is lacking. Therefore we report on the hardening with twist angle and on dislocation microstructures under twist loading and unloading for single crystals obtained by 3DDD [2].

[1] N. A. Fleck, G. M. Muller, M. F. Ashby, and J. W. Hutchinson. Acta Met. 42 (1994) 475.

[2] J. Senger, D. Weygand, O. Kraft, P. Gumbsch, *Dislocation microstructure evolution in cyclically twisted microsamples: a discrete dislocation dynamics simulation*, Modelling Simul. Mater. Sci. Eng. 19 (2011) 074004.

MM 6.2 Mon 11:45 H 0106

Existence of Two Twinning-Mediated Plastic Deformation Modes in Au Nanowhiskers — •Erik Bitzek[1], Andreas Sedlmayr[2], Daniel S. Gianola[3], Gunther Richter[4], Reiner Mönig[2], and Oliver Kraft[2] — [1]WW1, Department Werkstoffwissenschaften, Universität Erlangen-Nürnberg — [2]Institute for Applied Materials, Karlsruhe Institute of Technology — [3]Department of Materials Science and Engineering, University of Pennsylvania, Philadelphia, PA, USA — [4]Max-Planck-Institut for Intelligent Systems, Stuttgart

Single crystalline metallic nanowhiskers have lately attracted substantial interest due to their special mechanical properties. Here we report on in situ tensile experiments and molecular dynamics (MD) simulations on nominally defect-free single-crystalline Au nanowhiskers in [110] orientation. The room temperature experiments reveal strengths on the order of the ideal strength and plastic strains of up to 12%; a direct result of deformation twinning that is shown to govern the plastic flow. This is in clear contrast to the situation in coarse-grained fcc metals, where twinning is only observed at very low temperatures or at very high strain rates. The in situ and post mortem electron microscopy observations furthermore show two broad classes of deformation morphologies that correlate with distinct stress-strain responses. MD simulations show that the mechanism of twin growth can change from layer-by-layer propagation to parallel and accelerated formation of coalescing nanotwins.

MM 6.3 Mon 12:00 H 0106

Nano mechanical surface properties of the ferromagnetic shape memory alloy Ni-Mn-Ga — •Alexander Malwin Jakob and S.G. Mayr — Leibniz-Institut für Oberflächenmodifizierung, Translationszentrum für regenerative Medizin und Fakultät fuer Physik und Geowissenschaften der Universität Leipzig, 04318 Leipzig

During the last two decades, the wide field of so called "smart materials" attracted more and more interest in solid state physics. Ni-Mn-Ga, a ferromagnetic shape memory alloy (FMSM) - well known for its strong magneto-elastic coupling - yields high reversible strains up to 10% at external magnetic fields around 1 T [1]. Despite intensive investigations, nano scale processes causing magnetic shape memory effect still call for more detailed observation. Epitaxial grown 14M Ni-Mn-Ga thin films by magnetron sputtering are scope of our work. We investigate local indentation module M by means of contact resonance atomic force microscopy (CR-AFM) [2,3]. Experimental data are compared to theoretical predictions based on density functional theory (DFT). A discussion in context of super elasticity and phase transformations is given. This project is funded by the German BMBF, PTJ-BIO, Grant Number: 0313909

[1] Sozinov A., Likhachev A.A., Lanska N., and Ullakko K., Appl. Phys. Lett. Vol. 80, no. 10 (2002)

[2] Rabe U., Arnold W., Appl. Phys. Lett. Vol.64, P1493-1495 (1994)

[3] Yamanaka K., Ogiso H., Kolosov O., Appl. Phys. Lett., Vol.64, P178-180 (1994)

MM 6.4 Mon 12:15 H 0106

ab initio study of the mechanical shear behavior of Al with and without normal stresses — •Xueyong Pang, Rebecca Janisch, and Alexander Hartmaier — ICAMS, Bochum, Germany

To investigate the mechanical shear properties of interfaces in metals we have determined the gamma-surfaces of different special tilt and twist grain boundaries in aluminum by means of ab-initio calculations. From the gamma-surfaces we obtained minimum energy paths and barriers, as well as the theoretical shear strength. For the [110] tilt grain boundaries, the theoretical shear strength scales with the height of the slip barrier and exhibits a relation with the misorientation angle: the closer the angle to 90°, the higher the shear stress. To estimate the effect of full atomic relaxation, we carried calculations of the theoretical shear strength of Al single crystals in the (111) plane by different deformation methods. To investigate the influence of normal stresses on the shear behavior of Al, we also performed a series of combined normal/shear calculations on single crystal Al and grain boundaries. The critical shear strength follows the linear relationship with the normal stress; the critical shear strength decreases with the compression stress decreases and the tensile stress increases.

MM 6.5 Mon 12:30 H 0106

Ultrasensitive detection of biomolecules using Al nanostructures as SERS substrates — •Shankar Kumar Jha[1], Yasin Ekinci[1,2], and Jörg F. Löffler[1] — [1]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — [2]Paul Scherrer Institute, 5232 Villigen-PSI, Switzerland

Surface-enhanced Raman scattering (SERS) is an important technique for detecting molecules at low concentrations. The commonly used excitation sources are visible and near-infrared lasers since the frequently used SERS substrates support strong localized surface plasmon resonances (LSPR) at these wavelengths. Most of the biologically important molecules exhibit strong absorption in the deep-ultraviolet (DUV) wavelength region, giving rise to resonance Raman effect. Thus, apart from the increased Raman cross-sections and elimination of the prevalent fluorescence background, the use of DUV excitation would offer the possibility of combining the advantages of resonance Raman and SERS effects leading to surface-enhanced resonance Raman scattering (SERRS). We explore the use of designed aluminum nanoparticles as SERS substrates in the DUV region. The nanoparticle arrays fabricated over large areas using extreme-ultraviolet interference-lithography (EUV-IL) exhibit sharp and tunable LSPR in the UV and DUV wavelength ranges and allows for reproducible enhancement of Raman signal from molecules coated on these arrays. We demonstrate ultrasensitive and real-time analytical detection of biomolecules using these designed Al nanostructures as SERS substrates.