MM 5: Mechanical Properties

Mechanical Properties I and II

Time: Monday 10:15–13:00 Location: H46

MM 5.1 Mon 10:15 H46

Grain structure and mechanical properties of the Cu-Al hybrid materials processed by High Pressure Torsion Extrusion — Dayan Nugmanov, Roman Kulagin, Horst Hahn, and •Yulia Ivanisenko — Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), 76021 Karlsruhe, Germany

A comparative analysis of the microstructure and mechanical properties of Cu-Al hybrid samples with three different geometry configurations processed by High Pressure Torsion Extrusion (HPTE) had been performed. The HPTE technique allows to achieve large strains (up to 30) during just one pass in large-scale rod specimens with the diameter of 10 mm and the length of 35 mm. Room temperature tensile tests had shown an interesting two-stage mechanical behavior correspondent to the Cu-matrix and Al-wires tension processes. It was found that Al wires embedded in the ultrafinegrained (grain size less than one micrometer) Cu matrix got thinned as a result of HPTE, upon that wire thickness depends on its distance from the sample center. In specimen areas corresponding to the middle-radius initially one mm in diameter wires were thinned to the tapes with the thickness of 20-30 micrometers, whereas in the edge areas their thickness was two-three micrometers, which reflects the strain gradient at HPTE.

MM 5.2 Mon 10:30 H46

Plastic deformation of tungsten due to deuterium plasma exposure: Insights from micropillar compression tests — •Xufei Fang[1], Marcin Rasinski[2], Arkadi Kreter[2], Christoph Kirchlechner[1], Christian Linsmeier[2], Gerhard Dehm[1], and Steffen Brinckmann[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — [2]Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

The understanding of hydrogen embrittlement in metals is of importance for the failure prediction in components. Previous nanoindentation tests have shown that exposure to deuterium (D) plasma causes a decrease in pop-in load and an increase in hardness of tungsten. In this work, we use micropillar compression to investigate the plastic deformation and apparent strain hardening of tungsten exposed to D. In comparison to reference pillars, the pillars tested after exposure showed an increased apparent strain hardening rate as well as an increased multitude of slip traces. These outcomes are attributed to the presence of D that impedes the dislocation motion. Different loading rates in micropillar compression shed light on the competing mechanisms of dislocation and D mobility.

MM 5.3 Mon 10:45 H46

Mechanical properties of CrN-based nitride superlattices from ab inito calculations — •Lukas Löfler[1], Paul Heinz Mayerhofer[2], Matthias Bartosik[2], and David Holec[1] — [1]Montanuniversität Leoben, Leoben, Austria — [2]TU Wien, Vienna, Austria

Thin film coatings are used to protect surfaces of tools and components from harsh environmental and/or though pplication conditions. Next to changing the composition, a new way to tune material properties is to carefully create a microstructural design for the material. The simplest way are (semi-) coherent multilayers with a bi-layer period in the nm range. At certain thicknesses the materials show a significant increase in hardness and fracture toughness, two material properties relevant for many applications.

At such small scales the interface has an increasing influence on the overallproperties of the material. Density Functional Theory (DFT) is a potent technique to describe these superlattices and investigate their mechanical properties. CrN, a common coating material, was paired with AlN and TiN to form superlattices. At first, the elastic constants of different interface orientations were determined. Further, the critical tensile strength at and near those interfaces were calculated. To correlate the results to experiments, the KIC values in and perpendicular to the interface directions were calculated.

MM 5.4 Mon 11:00 H46

Effect of grain boundary morphology on crack propagation behaviour in Tungsten — •Shivraj Karewar and Erik Bitzek — Friedrich-Alexander Universität Erlangen-Nürnberg (FAU), Materials Science & Engineering, Institute I

Grain boundaries (GBs) in metals are commonly seen as preferential sites for crack nucleation and propagation. It has been shown that the atomic arrangements at GBs can affect the crack propagation [J. J. Möller, E. Bitzek, Acta Mat., 73, 2014, 1]. The atomic arrangement, in turn, depends on the misorientation, the GB plane, but also on GB defects like ledges and consequently on GB curvature.

Here we present the results of atomistic fracture simulations along tilt GBs in Tungsten. Crack propagation was studied for planar GBs of identical misorientation but different plane normals, as well as for curved GBs containing locally the same GB planes. Crack propagation for different GB misorientations were also investigated. In addition to quasi 2D simulations with minimal crack front length, simulations of extended crack fronts interacting with localized GB protrusions were performed. The results are discussed in terms of the plane-dependent GB energy, fracture surface area and the local stress state at GB defects.

MM 5.5 Mon 11:15 H46

Molecular dynamics investigation of size effects in lamellar γ-based TiAl alloys — •Ashish Chauniyal, Alexander Hartmaier, and Rebecca Janisch — ICAMS,Ruhr-Universität Bochum

Two-phase γ-based TiAl alloys with a lamellar microstructure are interesting candidates for high temperature structural applications, due to a beneficial combination of creep resistance and fracture toughness. These microstructures consist of the α_2-Ti_3Al and γ-TiAl phases, which can be as finely spaced as several tens of nanometers. The thickness and distribution of these phases in such nano-lamellar alloys is a dominant factor dictating their hardness, which increases with decreasing lamellae spacing. However, nanoindentation tests are limited by the indenter size which indents over several lamellae simultaneously and provides only an averaged value of local hardness. Furthermore, the dynamics in nano scale is hard to capture and is mostly speculative based on pre- and post-indentation images. Using large scale atomistic simulations, indents can be made on individual lamellae using small indenters, which allows us to decouple the individual influence of lamella thickness, spacing and lamella phase on the hardness of the samples. In this study we carry out molecular dynamics nanoindentation simulations to identify the origins of the experimentally observed size effects. Furthermore, we focus on the evolution of dislocation activity underneath the indenter and correlate it with local and average hardness.

15 min. break

MM 5.6 Mon 11:45 H46

Influence of Post Annealing on The Microstructure and Mechanical Properties of CuSn4/Fe Nanolaminates produced by ARB — •Maher Ghanem, Benoit Merle, Heinz Werner Höppel, and Mathias Göken — Friedrich Alexander Universität (FAU)_Lehrstuhl WW1: Allgemeine Werkstoffeigenschaften

The accumulative roll bonding (ARB) process has been applied to produce laminates with a layer thickness in the submicron to nanometer range. CuSn4/Fe nanolaminates with alternating layers of CuSn4 and Fe (99.88%) were produced by roll-bonding with 50% reduction and annealing at 400 *C following each pass. The rolling was repeated 14 times to achieve a layer thickness of about 100 nm. These nanolaminates were post annealed at different temperatures and the changes in their microstructure and mechanical properties as the number of ARB passes increased were observed. The microstructure was evaluated by means of backscatter electron (BSE) imaging and the mechanical properties of the nanolaminates were investigated through tensile and nanoindentation tests in order to observe the changes both locally and globally. It was found that the strength of the laminated composite could increase by a factor of about 2.5 times compared to single components. This increase in strength is discussed in terms of microstructural and phase interface contributions.

MM 5.7 Mon 12:00 H46

Adhesive wear mechanisms in the presence of weak interfaces — •Tobias Brink and Jean-François Molinari — Civil Engineering Institute and Institute of Materials Science and Engineering, EPFL, Lausanne, Switzerland

Despite the relevance of wear in many engineering applications, our understanding of the connection between mechanisms at the nanoscale and the observed wear rates of contacting parts at the macroscale remains limited. Recent work in our group has therefore focused on physics-based models of adhesive wear mechanisms, identifying a material-dependent critical length scale for wear particle formation [1]. Upscaling of these findings, though, still remains challenging [2]. One problem is that only strong adhesive bonds between contacting solids were considered. In the present contribution, we therefore extent this framework to include weaker interfaces, which are expected at typical contacts due to lattice mismatch, surface passivation, or lubrication. We use atomistic simulations on an amorphous model material to propose a mechanism map based on material properties and local contact geometry for wear particle formation and surface damage at the single-asperity scale. Our results imply that the local slopes of rough surfaces govern a transition from asperity collisions with plastic damage and wear particle formation at high roughness to slip without significant damage for flatter surfaces, comparable to a run-in process.

[1] Aghababaei, Warner, Molinari, Nat. Commun. **7**, 11816 (2016)
[2] Frérot, Aghababaei, Molinari, JMPS **114**, 172 (2018)

MM 5.8 Mon 12:15 H46

Electro-chemo-mechanical coupling of nanoporous gold at the microscale — •Yijuan Wu[1], Jürgen Markmann[1,2], and Erica Thea Lilleodden[1,3] — [1]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — [2]Institute of Materials Research and Technology, Hamburg University of Technology, Hamburg, Germany — [3]Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany

The effect of variation of electrode potential on the micro-mechanical behavior of nanoporous gold (NPG) was investigated by in situ micro-compression in an electrochemical environment. Micro-pillars of NPG were produced by focused ion beam milling and then mechanically tested in an electrolyte using a nanoindenter equipped with a flat punch. Using a novel loading profile, the contribution to the measured displacement due to the actuation could be decoupled from the compression-induced deformation. The electro-chemo-mechanical coupling resulted in a considerable increase in the strength of the pillars when surface adsorption occurred, i.e. under positive applied potential, and the stress response to potential jumps was found to be fast and reversible.

MM 5.9 Mon 12:30 H46

Verifying Larché-Cahn theory by measuring open-system elasticity of nanoporous palladium(-gold)-hydrogen — •Shan Shi[1,2], Jürgen Markmann[1,2], and Jörg Weissmüller[2,1] — [1]Institut für Werkstoffforschung, Werkstoffmechanik, Helmholtz-Zentrum Geesthacht, Geesthacht — [2]Institut für Werkstoffphysik und -technologie, Technische Universität Hamburg, Hamburg

Monolithic samples of nanoporous metals are suitable for studying the mechanical behavior of nanostructured metals via conventional, macroscale mechanical testing approaches. Here, we synthesized monolithic nanoporous palladium (np Pd) and palladium-gold (np Pd-Au) samples with ligament sizes below 10 nm, which allow fast hydrogen redistribution across their diameter when stress gradients are induced by bending. The corresponding variation of the Young's modulus during hydrogen absorption/desorption is measured by a dynamic mechanical analyzer. It is found that hydrogen sorption enables more than 30% reversible compliance variation in np Pd. Moreover, the redistribution of hydrogen, i.e. the change of local hydrogen concentration inside the ligaments, during the deformation causes an additional reduction of the effective elastic coefficients in the single-phase regime of Pd(-Au)-H at low hydrogen concentration. The measured Young's modulus shows excellent agreement with the prediction by the Larché-Cahn theory of open-system elasticity.

MM 5.10 Mon 12:45 H46

Ferroelectric fracture ratchet effect caused by flexoelectricity — •Kumara Cordero-Edwards[1,2], Hoda Kianirad[3], Carlota Canalias[3], Jordi Sort[4,5], and Gustau Catalan[1,5] — [1]Catalan Institute of Nanoscience and Nanotechnology (ICN2), Barcelona, Catalonia — [2]DQMP, University of Geneva, Geneva, Switzerland — [3]KTH-Royal Institute of Technology, Stockholm, Sweden — [4]Universitat Autònoma de Barcelona (UAB), Bellaterra, Spain — [5]Institució Catalana de Recerca i Estudis Avançats (ICREA), Barcelona, Catalonia

The propagation front of a crack generates large strain gradients and it is therefore a strong source of gradient-induced polarization (flexoelectricity). Fracture fronts generate flexoelectric fields that have an energy cost which, in turn, affects the mechanical response of materials. In ferroelectrics, this cost depends on the ferroelectric polarity. Therefore one can change the fracture toughness of a ferroelectric by switching its polarization.

Our work demonstrates experimentally that, as a consequence of flexoelectricity, crack propagation is promoted or diminished when directed parallel or antiparallel to the ferroelectric polarization, respectively. In addition, we have studied flexoelectrically induced domain switching around the crack, and showed that crack-induced flexoelectric switching is a contributor to the toughening of ferroelectrics with polarization antiparallel to the crack. The discovery of crack propagation asymmetry implies that fracture physics cannot be assumed to be symmetric in polar materials, and it demonstrates that flexoelectricity must be incorporated in any realistic model.