MM 23: Mechanical Properties II

Time: Tuesday 11:45–13:15 Location: H52

MM 23.1 Tue 11:45 H52

Dislocation structure and ordering effects in high entropy alloys — •Leonie Koch, Alexander Stukowski, and Karsten Albe — FG Materialmodellierung, FB Materialwissenschaft, Technische Universität Darmstadt, Germany

High entropy alloys, mixtures of least five elements, have recently attracted considerable attention in the field of high-performance materials. It is assumed that a high configurational entropy stabilizes solid solution states at low temperatures and simultaneously avoids the formation of brittle intermetallic phases. These structural simple solid solutions exhibit a considerable strength, while preserving sufficient ductility. Nevertheless, there has been some disagreement about the high entropy effect on phase formation and stability and chemical ordering instabilities in N-component alloys have not yet been clarified for a variety of alloy systems. Therefore, we investigate the competing effects of entropy and enthalpy with decreasing temperatures by using variance-constraint semi-grand canonical Monte Carlo simulations and subsequently quantify short-range order. We further show how inherent lattice strains in atomic-scale composites affect dislocation motion under external stress at different temperatures.

MM 23.2 Tue 12:00 H52

Embryonic cracks at grain boundaries in bcc W and Fe: an atomistic study — •Johannes J. Möller and Erik Bitzek — Friedrich-Alexander-Universität Erlangen-Nürnberg, Department of Materials Science and Engineering, Institute I, Erlangen, Germany

Advancing our understanding of grain boundary (GB) fracture is key for a variety of engineering problems spanning from brittle intergranular fracture of polycrystalline components to the failure of microelectromechanical devices at single GBs. GB cracks are often assumed to be infinitely long and straight. At the very beginning of their existence, however, embryonic cracks are of nano-scale dimensions and have strongly curved crack fronts. Until now, the effect of crack-front curvature on the elementary crack-tip processes has not been studied in detail.

Here, we report on our recent large-scale molecular dynamics simulations of penny-shaped cracks at five GBs in the bcc metals W and Fe. The observed crack-tip processes ranged from purely brittle bond breaking to purely ductile emission of deformation twins. The evolution of crack-tip plasticity is characterized by dislocation emission from growing twins and transmission of the nucleated dislocations through GBs. Our simulations indicate that the initial fracture event at penny-shaped crack fronts can be predicted by analyzing the results for straight cracks. The characteristic crack-tip processes, on the other hand, were not observed in such quasi-2D simulations. This highlights the importance of 3D modeling of cracks to obtain a deeper mechanistic understanding of the ongoing crack-tip processes.

MM 23.3 Tue 12:15 H52

Push-Out Verhalten von Wolfram-Faserverstärktem Wolfram — •Bruno Jasper[1], Stephan Schönen[2], Jan W. Coenen[1], Till Höschen[3], Johann Riesch[3], Rudolf Neu[3,4] und Christian Linsmeier[1] — [1]FZ Jülich GmbH, IEK4 - Plasmaphysik, Jülich, GER — [2]FZ Jülich GmbH, ZEA1 - Engineering und Technologie, Jülich, GER — [3]IPP, Garching, GER — [4]TU München, Garching, GER

Mit seinen vorteilhaften Eigenschaften im Bezug auf z.B. Wasserstoffrückhaltung oder Erosion durch Plasma ist Wolfram (W) ein Kandidat für Komponenten für die erste Wand zukünftiger Fusionskraftwerke. Der große Nachteil bei der Verwendung von W besteht jedoch in seiner hohen Spröd-Duktil Übergangstemperatur. Um diesen Nachteil zu umgehen wird ein Wolfram-Faserverstärkter Wolfram (W_f/W) Kompositwerkstoff entwickelt. Dieser besteht aus einem, mit einer Zwischenschicht (Interface) versehenen, W-Draht und einer W-Matrix. Wird ein Riss im Material initiiert, ist es auf Grund des Interfaces möglich, dass extrinsisch-zähigkeitssteigernde Mechanismen wirken können. Somit wird die Rissspitzenenergie reduziert und ein pseudoduktiles Verhalten erreicht.

Um ein besseres Verständnis dieser Mechanismen auf mikroskopischer Ebene aufzubauen wurden umfangreiche Push-Out Tests an dünnen Einzelfaser W_f/W Proben durchgeführt. Die experimentellen Ergebnisse, welche den Einfluss von Probengeometrie, Probenherstellung und Versuchsaufbau beleuchten, werden mit entsprechenden Simulationsarbeiten verglichen und vorgestellt.

MM 23.4 Tue 12:30 H52

Sequence of microstructure evolution processes in steel under tribological loading — •Christian Greiner, Karsten Wolff, Daniel Braun, Zhilong Liu, and Johannes Schneider — KIT, Kaiserstrasse 12, 76131 Karlsruhe

The exact evolution of a material's microstructure under tribological loading is of great importance for both materials physics and tribology. There is however a significant lack of knowledge about the elementary mechanisms of microstructure evolution under tribological load as well as their kinetics. Therefore, the microstructure evolution of steel C85 pellets sliding against steel 100Cr6 disks is characterized after different numbers of acceleration-deceleration cycles. Focused ion beam cross-sections are prepared along the sliding direction. Two tribologically modified surface layers are found: One with bent grain boundaries and one of nanocrystalline nature. We hypothesize that the second layer is formed by breaking down the most bent regions of the first one when a critical grain boundary bending angle is reached and then consumes it from the top. A model originally developed for High Pressure Torsion (HPT) was successfully applied to estimate the thickness of the fine-grained layer and the applied shear strain.

MM 23.5 Tue 12:45 H52

How ligament connectivity determines stiffness of nanoporous gold? — •Bao-Nam Ngô[1,2], Benedikt Roschning[3], Alexander Stukowski[2], Jürgen Markmann[1,3], Karsten Albe[2], and Jörg Weissmüller[1,3] — [1]Institut für Werkstoffforschung, Werkstoffmechanik, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — [2]Technische Universität Darmstadt, Fachbereich Material- und Geowissenschaften, Fachgebiet Materialmodellierung, Darmstadt, Germany — [3]Institut für Werkstoffphysik und Werkstofftechnologie, Technische Universität Hamburg-Harburg, Hamburg, Germany

We present a study of the deformation-induced changes of ligament connectivity and its influence on the elasticity of nanoporous gold - a promising material for applications in actuation, catalysis and sensing, as well as a model candidate for study of mechanics at the nanoscale. Using molecular dynamics, a computer sample created by spinodal decompostion was uni-axially deformed in a load/unload sequence. A surface reconstruction algorithm was employed to provide necessary information for calculating genus density and its changes during the plastic deformation. The results were then cast against corresponding changes of the elastic modulus. We also performed Finite Element Analysis on some deformed structures, using the reconstructed surfaces as initial structures in order to get a reference which is not influenced by size and interface effects. While our study reveals a strong influence of the ligament connectivity on the elastic behavior of nanoporous gold, other factors must be taken into account to explain its exceedingly compliant behavior.

MM 23.6 Tue 13:00 H52

Correlation between elasticity and stability in refractory alloys — •Sandra Hoppe[1], Sascha B. Maisel[2], and Stefan Müller[1] — [1]Institute of Advanced Ceramics, Hamburg University of Technology, Hamburg, Germany — [2]Max-Planck Institut für Eisenforschung, Düsseldorf, Germany

Varying an alloy's concentration or alloying constituents strongly influences its structural and mechanical properties. Modern simulation methods like density functional theory (DFT) in combination with the cluster expansion (CE) make the whole configuration space accessible. Recent results for several face-centered cubic (fcc) binary metal alloys [1] suggest a linear correlation between thermodynamic stability and elastic properties at a fixed stoichiometry. This study aims to investigate the generality of these findings by considering a similar correlation for the binary body-centered cubic (bcc) refractory alloy systems Ta-W and Mo-Nb. For this purpose, formation enthalpies as well as the symmetrically averaged elastic constants $\overline{c_{11}}$ and $\overline{c_{44}}$ are expanded via a CE fit with DFT input. Interestingly, the shear constant $\overline{c_{44}}$ shows an opposing trend to that observed for fcc alloys in certain concentration regimes. This phenomenon is discussed with regard to an anomalous behavior of $\overline{c_{44}}$ with varying alloy concentration, temperature or pressure [2,3].

[1] S. B. Maisel, M. Höfler, and S. Müller. *Nature* **491** (2012) 740.
[2] K. W. Katahara *et al. J. Phys. F: Met. Phys.* **9** (1979) 773.
[3] C. E. Anderson and F. R. Brotzen. *J. Appl. Phys.* **53** (1982) 292.