MM 64: Mechanical Properties: Plasticity, fracture, fatigue, wear - II

Time: Thursday 17:30–19:00 Location: IFW B

MM 64.1 Thu 17:30 IFW B

Can machine learning be used to extract single phase properties based on nanoindentation mapping? A case study in steels — •Robin Jentner[1], Kinshuk Srivastava[2], Bastian Philippi[2], Christoph Kirchlechner[1], and Gerhard Dehm[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — [2]AG der Dillinger Hüttenwerke, 66763 Dillingen, Germany

Advanced high strength steels exhibit an intricate microstructure comprising of several different phases and interfaces that determines the mechanical behavior of the bulk material. In order to examine the mechanical behavior of each individual phase, micro pillar compression tests have been used. However, micro pillar compression is tedious and time consuming. In this work, we explore the capability of high throughput nanoindentation combined with k-means clustering to determine the mechanical properties of each single phase.

We have trained first the k-means clustering method with a two-phase laboratory sample which was finally applied to a HSLA bainitic steel consisting of three different phases. The clustering revealed two to three clusters in the first case and at least five clusters for the bainitic steel. To unravel the origin of the additional clusters we have performed correlative microscopy and found that indents close to grain or phase boundaries are responsible for them. Based on the obtained results we conclude that analyzing the mechanical properties of complex bulk materials by k-means clustering provide a suitable microstructural characterization method, which will be discussed in the talk.

MM 64.2 Thu 17:45 IFW B

Atomistic and continuum simulation of brittle and ductile crack in titanium aluminide single and bi-crystals — •Anupam Neogi, Alexander Hartmaier, and Rebecca Janisch — ICAMS, Ruhr-Universität Bochum, Germany

Ti-Al alloys are well known for their excellent mechanical properties. However, they often exhibit low-ductility, which leads to in-service brittle failure. The fracture behavior of metallic materials is primarily governed by the competition between emission of dislocations and Griffith cleavage at the crack tip. In two-phase Ti-Al however, this simple picture is questionable. Here the anisotropy of the major phases, γ-TiAl and α_2-Ti_3Al, with a limited number of slip systems, leads to complex crack propagation mechanisms.

We investigate crack propagation under mode I loading in single-crystal γ and α_2 Ti-Al, as well as at γ/γ interfaces, using anisotropic linear elastic fracture mechanics (LEFM) and atomistic simulations. The latter show a significant directional dependence of crack tip behavior. For instance, a (111)-crack in γ-TiAl propagates by Griffith cleavage along $[\bar{2}11]$, but by dislocation emission along $[11\bar{2}]$. Basal cracks in α_2-Ti_3Al are generally assumed to propagate in a brittle manner, but we observe nucleation of dislocations if the crack propagates along $[10\bar{1}0]$. The complexity increases in the vicinity of γ/γ interfaces, in which the mechanism depends on the orientation of the crack plane with respect to the interface. Nevertheless, it is the remarkable conclusion of this study that the predictions of LEFM agree well - qualitatively and quantitatively - with atomistic simulations.

MM 64.3 Thu 18:00 IFW B

Multiscale quantum classical modelling of the interaction of crack systems with defects in diamond — •James Brixey and James Kermode — University of Warwick, Coventry, United Kingdom

Diamond is a material with many applications in industry and science, in particular for cutting and drilling. However, its brittle nature leads to catastrophic failure by fracture, and in order to reduce the probability of failure, it is important to understand as much about the atomic-scale details fracture as possible. Building on earlier work that found that individual boron impurities can form microscopic ridges in silicon, at certain crack speeds [Kermode et al, Nat. Comm (2013)], it is reasonable to postulate that single substitutional nitrogen in diamond might have interesting effects of a similar nature. In order to understand fracture of brittle materials, careful modelling of both the long-range stress field and the short-range bond breaking is required. To capture this, a multiscale (QMMM) model has been developed, using Density Functional Theory to accurately capture the activity far from equilibrium near the crack tip, whilst simultaneously capturing the elastic field interaction using an empirical interatomic potential. Preliminary results of our model will be presented, both for pure and defect containing diamond.

MM 64.4 Thu 18:15 IFW B

***In silico* experiments on mechanics of TiN/AlN superlattices: an MD study** — •Lukas Löfler[1], Matthias Bartosik[2], Paul Heinz Mayrhofer[2], and David Holec[1] — [1]Montanuniversität Leoben — [2]TU Wien

Nitride-based thin films are commonly used to protect components from harsh environments and high loading occurring in modern applications. A way to improve the mechanical properties of such coatings is to carefully design the microstructure. For instance, combining two materials in a coherent multilayer arrangement with layer thicknesses in the nm range (termed *superlattice*) can enhance both hardness and fracture toughness; two material properties that often seem to be mutually exclusive.

Utilizing molecular dynamics (MD), indentation and tensile loading simulations were performed to investigate the mechanical response of AlN/TiN superlattices on different loading scenarios. For the indentation, a spherical object was gradually moved into the coating displacing atoms. For the tensile loading, the atoms at the top and bottom of the coating were moved so to apply axial tension. For both setups, the forces, stresses and the nucleation of dislocations were analyzed. To gain more insight into the nucleation process of the dislocations, different cores and their structures were calculated for the most common slip systems.

MM 64.5 Thu 18:30 IFW B

Effect of lattice misfit on the deformation behaviour of two-phase lamellar TiAl alloys — •Ashish Chauniyal and Rebecca Janisch — ICAMS, Ruhr Universit
"at Bochum

Deformability and strength of two phase TiAl alloys strongly depends on the presence of different interfaces in their microstrucure. Two phase TiAl alloys consists of face centered tetragonal γ(TiAl) phase and hexagonal $\alpha_2(Ti_3Al)$ phase. The interfaces in lamellar alloys are either γ/γ or α_2/γ. Lattice misfits arise due to different crystal structures at α_2/γ interface or due to tetragonality at γ/γ interfaces. A coherent interface, with matching lattice points, leads to coherency stresses in lamellae, whereas a semi-coherent interface has misfit dislocations. Using molecular dynamics simulations we study the deformation behaviour of coherent and semi-coherent interfaces by carrying uniaxial tensile tests on bi-layer specimens of α_2,γ. We quantify the relation between volume fraction and coherency stresses in lamellae and distinguish the role of volume fraction and individual lamellar size on deformation behaviour. Coherency stresses in lamellae lead to early yielding of α_2,γ bilayers which could be the origins of the observed microplasticity in TiAl alloys. Furthermore, we show that misfit dislocations at the interfaces create local stress fluctuations within the lamellae, which in turn, lead to dislocation nucleation. Thus, we distinguish different dislocation nucleation mechanisms in coherent and semi-coherent interfaces in correlation with changing stress states caused due to lattice misfit.

MM 64.6 Thu 18:45 IFW B

Mechanical property gradients of spider attachment hairs — •Silja Flenner[1], Clemens Schaber[2], Imke Greving[1], Igor Krasnov[1], Manfred Burghammer[3], Martin Rosenthal[3], Stanislav Gorb[2], and Martin Müller[1] — [1]Helmholtz-Zentrum Geesthacht, Germany — [2]Institute of Zoology, Kiel University, Germany — [3]ESRF, Grenoble, France

The hairy attachment system of spiders enables these animals to walk upside-down on rough and smooth surfaces and support a multiple of the body weight without the use of glue. These outstanding biological structures comprise of pads including thousands of specially designed hairs that are made of composite materials consisting of proteins and reinforcing chitin fibres.

The technique of high spatial resolution mapping based on scanning X-ray nanobeam diffraction and small-angle scattering was used to study the hairy attachment system of spiders. Each point of a map

represents a structural parameter such as orientation or scattered intensity extracted from a diffraction pattern. Additional nanotomography measurements allows to correlate the structural parameters with 3D data. These techniques were combined with an in situ attachment/detachment procedure. The goal of our study is to gain an in-depth understanding of the structures and mechanical properties of single hairs during the attachment and detachment process to a surface.