

## MM 38: Mechanical Properties III

Time: Wednesday 16:30–18:00

Location: H16

MM 38.1 Wed 16:30 H16

**Statistical Dislocation Dynamics: Some Comments** — ●MARKUS HÜTTER — Polymer Physics, Department of Materials, ETH Zurich, CH-8093 Zurich, Switzerland

A statistical description of dislocation dynamics is examined from the perspective of nonequilibrium thermodynamics. Particularly, the evolution of the densities of different dislocation types is embedded into a macroscopic model for elasto-viscoplasticity. By this procedure, we discuss in detail the following points.

First, the motion of mobile dislocations is studied in order to formulate a constitutive relation for the plastic strain rate tensor in macroscopic viscoplasticity, also known as the plastic distortion rate tensor. We find a rigid connection between the Peach-Koehler force and the plastic strain rate tensor in terms of a tensorial Orowan equation. The thermodynamic driving force for dislocation motion, and for plastic flow, is identified. Specifically, a clear distinction is made between dislocation interactions and forces on dislocations due to macroscopic stress fields.

Second, we examine some frequently used reaction-type equations for mobile and immobile dislocations to model the ubiquitous strain-hardening. We demonstrate that a certain class of such models is in conflict with thermodynamic principles. The origin of this conflict is identified. Particularly, the absence of the reversal processes for any of the reactions is problematic and sharply contrasts to usual chemical reactions. Possible solutions for restoring the thermodynamic admissibility are discussed.

MM 38.2 Wed 16:45 H16

**Interface fracture simulation in lamellar TiAl crystals** — ●PAVEL LEIVA RONDA, KARSTEN DURST, FARASAT IQBAL, and MATHIAS GÖKEN — Institute of General Material Properties, Department of Materials Science and Engineering, University Erlangen-Nürnberg, Germany

A microscale fracture simulation has been applied to study the toughening of lamellar TiAl crystals through interface mechanisms. The crack growth at the weak  $\gamma$ -TiAl/ $\alpha_2$ -TiAl and  $\gamma$ -TiAl/ $\gamma$ -TiAl lamellar interfaces has been simulated by means of a finite element method using a cohesive modelling approach. The elasticity for  $\gamma$  and  $\alpha_2$  phases is assumed to be anisotropic while the plasticity model considers a continuum material with a proper homogenization of the two phases lamellar system. In this sense, the constitutive plastic behaviour is described by a two-dimensional plane stress Hill's model based on reported crystal plasticity calculations. Parametric studies have been performed to investigate the effect of cohesive parameters as the energy release rate and also the influence of residual stresses on the fracture behaviour. Furthermore, it has been analyzed the relationship between bulk and interface properties within the frame of the cohesive model for the TiAl lamellar crystals.

MM 38.3 Wed 17:00 H16

**Finite Auxetic Deformations of Plane Tessellations** — ●HOLGER MITSCHKE<sup>1</sup>, GERD E. SCHROEDER-TURK<sup>1</sup>, VANESSA ROBINS<sup>2</sup>, and KLAUS MECKE<sup>1</sup> — <sup>1</sup>Theoretische Physik, Friedrich-Alexander Universität Erlangen-Nürnberg, Staudtstr. 7B, 91058 Erlangen — <sup>2</sup>Applied Maths, School of Physics, The Australian National University, 0200 ACT, Canberra, Australia

We describe a systematic approach to study finite deformations of plane periodic symmetric skeletal structures or strut frameworks, consisting of stiff rods that pivot freely at the mutual joints. These skeletal structures are deformed by imposing a strain in one of the lattice directions and determining the response in the other lattice direction. A numerical Newton-Raphson scheme is used to find the deformation pathways that maintain constant strut lengths. The deformation behaviour is quantified by finite and instantaneous (or infinitesimal) Poisson's ratios  $\nu$  and  $\nu_{inst}$ . This analysis allows in particular the analysis of skeletal structures based on tessellations of the plane. Applied

to one- or two-uniform tessellations by regular or star polygons, this analysis reveals two as yet unknown structures with auxetic mechanisms. It also shows that a number of other periodic skeletal structures become auxetic at finite strain when retaining some or all symmetries during the deformation, some with Poisson's ratios below  $-1$ . The approach can be generalized to three-dimensional skeletal structures.

MM 38.4 Wed 17:15 H16

**Effective Elastic Moduli in Solids with High Density of Cracks** — ●ROBERT SPATSCHEK<sup>1</sup>, CLEMENS GUGENBERGER<sup>2</sup>, and EFIM BRENER<sup>2</sup> — <sup>1</sup>ICAMS, Ruhr-Universität Bochum — <sup>2</sup>IFF, Forschungszentrum Jülich

We investigate the weakening of elastic materials through randomly distributed circles and cracks numerically and compare the results to predictions from homogenization theories. We find a good agreement for the case of randomly oriented cracks of equal length in an isotropic plane-strain medium for lower crack densities; for higher densities the material is weaker than predicted due to precursors of percolation. For a parallel alignment of cracks, where percolation does not occur, we analytically predict a power law decay of the effective elastic constants for high crack densities, and confirm this result numerically.

MM 38.5 Wed 17:30 H16

**Simulation der Ermüdung von metallischen Werkstoffen durch ein granulares Modell** — ●JUDITH FINGERHUTH<sup>1</sup>, MATZ HAAKS<sup>1</sup>, GUNTER SCHÜTZ<sup>2</sup> und KARL MAIER<sup>1</sup> — <sup>1</sup>Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn — <sup>2</sup>Institut für Festkörperforschung, Forschungszentrum Jülich

Basierend auf der Idee des zellulären Automaten wird die Akkumulation offenen Volumens bei der Ermüdung eines Metalls mit einem mesoskopischen Modell simuliert. Der Kristall wird dabei als regelmäßige Anordnung von Kristallkörnern betrachtet, deren komplexe, individuelle Eigenschaften durch die skalaren Parameter Korngröße, Orientierung, mittlere Versetzungsdichte und Konzentration offenen Volumens repräsentiert werden. Die Versetzungsdichte erhöht sich in Abhängigkeit vom Spannungszustand des Korns, die Konzentration offenen Volumens erhöht sich nach dem Modell von Essmann, Gösele und Mughrabi und durch das Schneiden von Schraubversetzungen. Durch Kombination mit Finite-Elemente-Methoden lässt sich im Prinzip die Ermüdung einer Probe mit beliebiger Geometrie simulieren. Die Rechenzeit zur Simulation der eigentlichen Ermüdung einer Probe mit 10.000 Körnern über eine Million Zyklen auf einem einzelnen Arbeitsplatzrechner beträgt etwa eine Stunde.

MM 38.6 Wed 17:45 H16

**Performance optimized phase-field simulations of grain structures under the effect of mechanical forces** — ●ALEXANDER VONDROUS, MICHAEL SELZER, BRITTA NESTLER, and MARCUS JAINTA — Karlsruhe University of Applied Sciences, Moltkestr. 30, 76133 Karlsruhe

An extension of the phase-field model for polycrystalline materials is presented that incorporates the effect of mechanical forces (elasticity and plasticity) on the microstructure. We derive the set of dynamical equations and show simulations of micro cracks in grain structures under the influence of elastic stresses. Isotropic, linear elastic energies according to Hooke's law are applied in the bulk phase regions to account for the stress distribution. A new approach to describe small plastic deformations in the context of the phase-field method is based on ideal plasticity models by Tresca and von Mises criterions. We compute the wave equation of the displacement vector on a staggered grid. Modern parallel and adaptive techniques improve the performance of the numerical algorithms and allow to efficiently employ high performance clusters. As a long range objective, we aim to develop a simulation environment for microstructure formations during rolling and press hardening processes in manufacturing processes of metals.