MM 38: Topical Session: Fundamentals of Fracture - Atomistic Modelling

Time: Wednesday 15:00–16:15 Location: H4

Topical Talk MM 38.1 Wed 15:00 H4

Modelling fracture scattering by defects in brittle crystals — •Alessandro De Vita, James Kermode, Giovanni Peralta, Marco Caccin, and Zhenwei Li — King's College London, Physics Department, Strand, London WC2R 2LS, United Kingdom

We present the results of an atomistic modelling investigation of crack-defect interaction, using the "Learn On The Fly" (LOTF) hybrid multi-scale simulation scheme [1]. The scheme is particularly well-suited to incorporate machine-learning (ML) approaches based on the predictive inference of atomic forces, and has been previously used to model both "intrinsic" crack propagation instabilities [2] and the interaction of propagating cracks with defects such as dislocations and implanted ions [3].

Here, taking as a target system B-doped ultra-pure Si samples, we provide theoretical and experimental evidence suggesting that contrary to common wisdom, propagating cracks can be deflected by hitting a single, isolated impurity atom, yielding predictable patterns of macroscopic roughness on the cleavage surface.

[1] G.Csanyi, T.Albaret, M.C.Payne and A.De Vita, PRL 93, 175503 (2004); [2] J.R.Kermode, T.Albaret, D. Sherman, N. Bernstein, P.Gumbsch, M.C.Payne, G.Csanyi and A.De Vita, Nature 455, 1224-U41 (2008); [3]G.Moras, L.C.Ciacchi, C.Elsaesser, P.Gumbsch and A.De Vita, PRL 105, 075502 (2010);

MM 38.2 Wed 15:30 H4

Atomic scale modeling of damage evolution in high temperature ceramics — •Yuriy Natanzon, Denis Pilipenko, and Heike Emmerich — Lehrstuhl für Material und Prozessimulation, Universität Bayreuth, Nürnberger Straße 38, 95448 Bayreuth, Bayern

The fracture phenomenon is a major challenge for solid state physics and material science. Modelling of damage evolution is crucial for the design of advanced materials such as high temperature ceramics, which receive more attention due to increased demand for materials for extreme environments. Due to the resulting high thermal shock resistance, carbon is used in more than 40% of all fire-proof products worldwide to adjust their thermomechanical and chemical properties. For the development of "cleaner" fire-proof parts and the consequential avoidance of carbon, it is essential to understand how other materials can tailored to reach a comparable thermal shock resistance even under today's higher thermal shock stresses.

Here we present the results of atomic scale modeling of propagation of microcracks in such fire-proof ceramics by means of classical molecular dynamics with various semi-empirical interatomic potentials. The dependence of direction of crack and its speed on the various crystal orientations as well as the loading regime is calculated. and the role of charge transfer on the crack dynamics is analysed.

MM 38.3 Wed 15:45 H4

Atomistic Simulations of Cracks in α-Iron: 2D vs. 3D — •Johannes J. Möller and Erik Bitzek — Friedrich-Alexander-Universität Erlangen-Nürnberg, Department of Materials Science and Engineering, Institute of General Materials Properties, Martensstr. 5, 91058 Erlangen, Germany

Atomistic simulations play a crucial role in advancing our understanding of the crack tip processes taking place during fracture. As with all atomistic simulations, the results depend critically on the model of atomic interaction and on the boundary conditions. Here we present a systematic study of seven different embedded atom method (EAM) potentials applied to mode I cracks in α-iron and compare the results of straight crack fronts in quasi-two-dimensional (2D) set-ups with curved crack fronts in three-dimensional (3D) set-ups.

Infinitely long, straight crack fronts were studied in a cylindrical geometry where the atoms are displaced according to the anisotropic linear-elastic solution and periodic boundary conditions are applied along the crack front direction. Comparison of the fracture behavior and critical stress intensity factors to experimental data allows us to rank the potentials according to their capability to realistically model fracture in α-iron. The results of these quasi-2D simulations are compared to large-scale 3D molecular statics and -dynamics simulations of penny shaped cracks. The plastic deformation mechanisms and changes in crack morphology are analyzed in detail and related to the curvature of the crack front and the 3D simulation set-up. The results highlight the importance of 3D models to study microstructurally short cracks.

MM 38.4 Wed 16:00 H4

Studying Short Cracks with a 3D Multiscale Model — •Steffen Brinckmann — Max Planck Institut für Eisenforschung

Grooves and notches act as initiation sites for short cracks, which grow into size and lead to a failure of the structure. To understand the fundamentals of short cracks, a multiscale model is warranted, which accounts for fracture on the atomistic level, while covering plasticity on a micrometer length scale.

Multiple multiscale models exist, which cover these intrinsic length scales: atomistic separation by Molecular Dynamics and micrometer plasticity by Dislocation Dynamics. In the past, these models were restricted to two dimensional configurations, which limited their applicability and altered the fundamental deformation behavior of the metal.

In this contribution a three-dimensional, concurrent multiscale model of Molecular and Dislocation Dynamics is introduced and applied to microscale plasticity around a short penny-shaped notches, which is located at the free surface. Since this contribution is the first-time presentation of the three-dimensional model AtoDis, a full description of the mechanical model, especially at the interface is given.

The talk will close with remaining challenges in the current model and a general discussion about model verification, which is applicable to multiple of the currently developed multiscale models.