MM 15: Topical Session: Fundamentals of Fracture – Atomistic Studies of Fracture

Time: Tuesday 10:15–13:00 Location: SCH A 216

Topical Talk MM 15.1 Tue 10:15 SCH A 216

Multiscale Quantum-Atomistic and Atomistic-Continuum Modelling of Crack Propagation — •James Kermode — Warwick Centre for Predictive Modelling, School of Engineering, University of Warwick, Coventry, United Kingdom

I will review recent progress on the development and application of advanced algorithms to simulate chemomechanical systems where local chemistry and long-range stress are tightly coupled, e.g. at the tip of a propagating crack or the core of a dislocation. I will discuss two general approaches (i): hybrid quantum/classical approaches where bond-breaking is treated at the DFT level embedded within a large-scale classical atomistic model to capture elastic relaxation, including recent applications to tungsten [1] and diamond [2]; (ii) atomistic-to-continuum modelling for crack propagation, either through extracting effective continuum models from large-scale atomistic simulations of fracture [3], or by flexibly embedding an atomistic domain within a continuum model, using a new algorithm to compute bifurcation diagrams for fracture systems [4].

[1] P. Grigorev et al., arXiv:2111.11262 (2022); [2] J. Brixey, T. Cowie, A. Jardine and J. R. Kermode, In Prep (2022); [3] S. M. Khosrownejad, J. R. Kermode, and L. Pastewka, Phys. Rev. Materials 5, 023602 (2021); [4] M. Buze and J. R. Kermode, Phys. Rev. E 103, 033002 (2021)

MM 15.2 Tue 10:45 SCH A 216

Modelling Fracture in α-Iron via a Numerical-Continuation Scheme — •Lakshmi Shenoy[1], Albert Bartok-Partay[2], and James Kermode[1] — [1]Warwick Centre for Predictive Modelling, School of Engineering, University of Warwick, Coventry CV4 7AL, United Kingdom — [2]Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom

I will present results for the stability range of fracture in α-iron mapped using the numerical-continuation flexible boundary scheme (NCFlex) proposed by Buze et. al. [1]. The predictions by two new machine learning interatomic potentials for α-iron [2] - Gaussian approximation potential and atomic cluster expansion - will be compared with those by the classical embedded atom model [3]. From the bifurcation plots produced by NCFlex, the 0K energy barriers to brittle fracture propagation along different crystallographic planes in α-iron will be computed. Using these, a model for the temperature dependence of the brittle-to-ductile transition temperature of α-iron will be proposed, and validated against experimental results. Methods for extending this scheme to finite temperature energy barriers and interaction of the crack tip with point defects will also be discussed.

[1] M. Buze and J. R. Kermode, Phys. Rev. E 103, 033002 (2021) ; [2] Zhang, Lei, et al. arXiv:2208.05912 (2022) ; [3] Mendelev, M. I., et al. Phil. Mag. 83.35 (2003)

MM 15.3 Tue 11:00 SCH A 216

Revealing Atomistic Fracture in BCC Iron by Active Learning — Lei Zhang[1], Gabor Csanyi[2], Erik van der Giessen[1], and •Francesco Maresca[1] — [1]University of Groningen, Netherlands — [2]University of Cambridge, UK

Fracture is multi-scale process that originates from atomic-scale bond rupture and dislocation activity. A clear understanding of these processes is often lacking, because classical interatomic potentials (IAPs) for Molecular Dynamics simulations yield contradicting results that agree only partially with experiments. This is also due to the limited flexibility of their functional form, which is inadequate to describe the complex potential energy surface associated with fracture processes. Emerging machine learning (ML) IAPs allow near-quantum accuracy, based on density functional theory (DFT), but are orders of magnitude faster than DFT. In this work, we develop an active learning algorithm that enables the prediction of atomistic fracture mechanisms via the Gaussian Approximation Potential (GAP) approach. An existing DFT database for ferromagnetic bcc iron is first enriched with configurations that are relevant for the fracture process. Next, the active learning approach is applied to four crack systems, in which the maximum predicted per-atom error is reduced to 10 meV. The predicted critical stress intensity factors are compared with theory estimates, and the learning efficiency of the approach is analysed. Our work provides an active learning strategy for improving ML-IAPs for fracture, while revealing for the first time the atomic scale mechanisms that initiate fracture in iron with quantum accuracy.

MM 15.4 Tue 11:15 SCH A 216

Benchmarking of Tungsten Potentials using Blunted Cracks — •Tarakeshwar Lakshmipathy and Erik Bitzek — Department Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH

Blunted cracks can have radically different fracture behavior compared to their atomically sharp counterparts due to the additional degrees of freedom available to atoms at the crack tip surface. Simulating realistic notch or crack tip radii requires computationally inexpensive atomic interaction potentials. However, empirical potentials are known to show artefacts like the formation of planar faults at the crack tip due to unrealistic minima in their generalized stacking fault energies or fail to reproduce surface reconstructions. Such drawbacks could play an even larger role in blunted crack simulations than in typically studied sharp cracks due to additional surfaces at the crack tip. In this work, the fracture behavior and fracture toughness of some commonly used EAM potentials are benchmarked against density functional theory (DFT) simulations of blunted cracks in tungsten and compared to recently developed modified-EAM (MEAM), atomic cluster expansion (ACE) and bond order potentials (BOP).

15 min. break

MM 15.5 Tue 11:45 SCH A 216

Development of machine learning interatomic potentials for far-from-equilibrium states: a case study of deformation mechanisms in ceramics — •Shuyao Lin[1], Davide Sangiovanni[2], Lars Hultman[2], and Nikola Koutna[1] — [1]Technical University of Vienna, Institute of Materials Science and Technology, A-1060, Vienna, Austria — [2]Linköping University, Department of Physics, SE-58183, Linköping, Sweden

Besides the high chemical stability, the applications of ceramic-based materials into the coating technology require not only high strength but also ductility, a combination of properties necessary for material's resistance to crack growth. The mechanical properties of ceramic materials are dominated by both their movement and interactions. In this talk, we study mechanical response of selected ceramics, including transition metal diborides and nitrides. First, ab initio molecular dynamics simulations (AIMD) are employed to model tensile deformation along main crystallographic directions and under extreme high temperatures with fluid status. Then we develop machine learning interatomic potentials within the moment tensor potential (MTP) framework. The potentials are thoroughly tested and validated against AIMD stress-strain curves. With the aid of newly developed potentials, we carry out large-scale simulations during which the ceramics are continuously loaded and can shrink due to Poisson contractions. The observed deformation mechanisms are described and compared to those present in the small-scale training data.

MM 15.6 Tue 12:00 SCH A 216

Atomistic studies of crack tip twin-boundary interactions in lamellar TiAl alloys: Effect of misfit, misorientation and lamella spacing — Anupam Neogi[1,2] and •Rebecca Janisch[1] — [1]ICAMS, Ruhr-University Bochum, Germany — [2]ANSYS Inc., Pune, India

Nano-scale coherent twin boundaries can be an effective way in overcoming the strength-ductility trade-off of metals and their alloys. In this sense also twin boundaries in nano-lamellar lightweight Ti-Al alloys promise a great potential. Furthermore, the existence of three types of these twin boundaries with different misorientation and coherency state at the interface provide an excellent opportunity to study the effect of exactly these parameters in a realistic model system. To this end, we carried out molecular statics simulations to characterize the crack advancement at and across internal true-twins (TTs), rotational boundaries (RBs), and pseudo-twins (PTs) in lamellar γ-TiAl alloys, as well as crack propagation in fully lamellar structures.

It was confirmed that both interface type and spacing affect the fracture toughness and crack growth resistance. Furthermore, the crack tip mechanisms exhibit prominent sensitivity to the crack system and crys-

tallographic directions. For trans-lamellar cracks the tip shows plastic deformation and toughening at all interfaces. The overall fracture initiation toughness in a microstructure of TTs exhibits an increasing trend with decreasing lamellar size down to a critical thickness, below which the fracture toughness drops again. These and more phenomena and their origins will be discussed in the presentation.

MM 15.7 Tue 12:15 SCH A 216

Crack Dislocation Interactions in Tungsten — •Benedikt Eggle-Sievers and Erik Bitzek — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf

The fracture toughness of Tungsten at low temperature is critically influenced by its microstructure. Understanding the underlying crack-microstructure interactions is therefore necessary to model and predict failure. In order to gain insight into the interactions of dislocations with the crack-tip, large scale atomistic simulations are carried out. Dislocations of different character and Burgers vector are placed in the vicinity of a strain controlled crack geometry, resulting either in an attraction or repulsion of the dislocation. In the former case interactions can be observed in the course of the simulation, e.g. cross-slipping of screw parts, changes in crack front or crack plane as well as subsequent dislocation emission. Dependencies on the stress state, the crack system, dislocation type and distance between dislocation and the crack are investigated. The results are discussed with respect to mesoscale and continuum models for crack tip plasticity and fracture toughness.

MM 15.8 Tue 12:30 SCH A 216

Atomistic study of fracture in Laves phases — •Alireza Ghafarollahi and Erik Bitzek — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, Düsseldorf 40237, Germany

Laves phases are intermetallic phases with complex structures that exist in many alloys and have a pronounced impact on their mechanical properties. Although these materials often exhibit superior mechanical properties at high temperatures, their applications as structural materials are limited due to their intrinsic brittleness at ambient temperature. Therefore, understanding the fundamental fracture mechanisms in Laves phases is crucial for tailoring their mechanical properties. Here, with the aid of atomistic simulations, the fracture behavior in C14 and C15 Laves phases is explored using NbCr_2 and MgZn_2 as model systems. In particular, different crack systems are analyzed and the corresponding fracture toughnesses are computed and compared with the Griffith theory.

MM 15.9 Tue 12:45 SCH A 216

Tailoring negative pressure by crystal defects: Crack induced hydride formation in Al alloys — •Ali Tehranchi[1], Poulami Charaborty[1], Marti Lopez Freixes[1], Eunan McEniry[1], Baptiste Gault[1,2], Tilmann Hickel[1,3], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, D-40237 Düsseldorf, Germany — [2]Department of Materials, Imperial College, South Kensington,London, SW7 2AZ, UK — [3]Bundesanstalt für Materialforschung und -prüfung (BAM)

Climate change motivates the search for non-carbon-emitting energy generation and storage solutions. Metal hydrides show promising characteristics for this purpose. To enhance the formation and stability of such often highly volatile hydrides we have consider a novel concept: tailoring and employing the negative pressure of microstructural and structural defects to enhance H solubility and thus hydride formation. Using systematic ab initio and atomistic simulations, we demonstrate that an enhancement in the formation of hydrides at the negatively pressurized crack tip region is feasible by increasing the mechanical tensile load on the specimen. The theoretical predictions have been used to reassess and interpret atom probe tomography experiments for a high-strength 7XXX-aluminium alloy that show a substantial enhancement of hydrogen concentration at structural defects near a stress-corrosion crack tip. Based on these insights we derive strategies for enhancing the capability of metals as H-storage materials.