MM 21: Topical Session (Symposium MM): Fundamentals of Fracture

Interface Fracture and Atomistic Aspects I

Time: Tuesday 10:15–11:30 Location: TC 006

Topical Talk MM 21.1 Tue 10:15 TC 006

Comparison of interfacial fracture properties in molecular dynamics simulations: A primer on selecting grain boundary sets — •Remi Dingreville[1], Doruk Aksoy[2], and Douglas Spearot[2] — [1]Sandia National Laboratories — [2]Department of Mechanical Engineering, University of Florida

All grain boundaries are not equal in their predisposition for fracture due to the complex coupling between lattice geometry, interfacial structure, and mechanical properties.

This presentation will describe a methodology to isolate the role of grain boundary structure on interfacial fracture properties using atomistic simulations. Instead of commonly constructing sets of grain boundary models within the misorientation/structure space by simply varying the misorientation angle around a fixed misorientation axis, the proposed method creates sets of grain boundary models by means of isocurves associated with important fracture-related properties of the adjoining lattices. Such properties may include anisotropic elastic moduli, the Schmid factor for primary slip, and the propensity for simultaneous slip on multiple slip systems. This approach eliminates the effect of lattice properties from the comparative analysis of interfacial fracture properties and thus enables the identification of structure-property relationships for grain boundaries. As an example, this methodology is implemented to study crack propagation along Ni grain boundaries. Segregated H is used as a means to emphasize the role of the grain boundary structures while keeping lattice properties fixed.

MM 21.2 Tue 10:45 TC 006

Intergranular fracture prediction via multi-scale simulations — •Bertrand Sicaud[1,3], Laurent Van Brutzel[2], and Maxime Sauzay[1] — [1]DEN- Service de Recherches Métallurgiques Appliquées (SRMA), CEA, Université Paris-Saclay, F-91191, Gif-sur-Yvette, France — [2]DEN- Service de la Corrosion et du Comportement des Matériaux dans leur Environnement (SCCME), CEA, Université Paris-Saclay, F-91191, Gif-sur-Yvette, France — [3]Universités Paris-Sorbonne - UPMC, 75005 Paris, France

Observations of intergranular fracture initiation during slow strain rate tests highlight two relevant mechanisms occuring at grain boundaries (GB): stress concentrations induced by the impact of slip bands and selective internal oxidation in water environment.

The pile-up theory modeling a slip band as a slip plane of negligible thickness in a continuum elastic medium is generaly used with the Griffith criterion. However this approach leads to large underestimation of the remote stress to GB fracture.

Slip band of finite thickness (20-200 nm) inducing more realistic singularities are investigated by using crystalline finite element calculations. A new approach using quantized fracture mechanics in conjunction with a double criterion permits to deduce a model of intergranular crack initiation. This multi-scale analytical model is used with molecular dynamics results of oxide grain boundaries decohesions for assessing the oxidation embrittlement of the interface. An extensive application of the model is carried out for numerous materials. Predictions are in good agreement with experimental results.

MM 21.3 Tue 11:00 TC 006

Exploring the mechanisms of Pellet-Cladding Interaction with atomistic simulation — •Adam Plowman, Conor Gillen, Alistair Garner, Philipp Frankel, and Christopher Race — University of Manchester, Manchester, United Kingdom

Failure of fuel rods in light water nuclear reactors via the Pellet-Cladding Interaction (PCI) is thought to be driven by Stress Corrosion Cracking (SCC), induced by aggressive fission products such as iodine. Empirical observations of PCI together with a limited mechanistic understanding of the phenomenon has led to stringent limits on operational parameters. An improved understanding of PCI would allow these limits to be relaxed and enable reactors to respond to energy demand changes more quickly, without compromising safety. Flexible power manoeuvring is critical to successfully combining nuclear power with fluctuating sources of renewable energy. In tandem with new experimental observations, we are using atomistic simulation to improve our mechanistic understanding of PCI. We present a systematic study of zirconium grain boundary properties, including cleavage energies, undertaken using density functional theory. We have further studied the thermodynamics of impurities (including iodine) in these boundaries and their effect on grain boundary cohesion. We compare our results with new experimental data on iodine-induced SC cracks in commercial Zr alloys.

MM 21.4 Tue 11:15 TC 006

Predicting mechanical properties of carbide-metal interfaces from first principles — •Elric Barbé[1,2], Chu-Chun Fu[2], and Maxime Sauzay[1] — [1]CEA, DEN, Service de Recherches Métallurgiques Appliquées, F-91191, UPSay, Gif-sur-Yvette Cedex, France — [2]CEA, DEN, Service de Recherches de Métallurgie Physique, F-91191, UPSay, Gif-sur-Yvette Cedex, France

The cavity initiation observed in ductile, brittle and intergranular creep damages is often explained by a fracture of interface between carbide and metallic lattices. Understanding the mechanisms of fracture allows the prediction of the cavity density as a function of applied strain, which law strongly affects the damage evolution. This study focuses on interfaces between a metallic matrix (Fe, Ni) and a representative carbide: M23C6 . Surface, interface and fracture energies are calculated via DFT based on chemical potential analysis. Then, interfacial fractures stresses are estimated by the UBER (Universal Binding Energy Relation) model and compared with good correlation to the results of fully-DFT simulations of tensile test carried out using various methodologies. We investigate the dependence of the interfacial mechanical behavior on chemical compositions, crystallographic structures and magnetic orderings. The predicted fracture stresses of coherent interfaces range between 14 and 20 GPa. Then, the effects of some incoherent interfaces are investigated. The resulting critical stress is about two times smaller, which is consistent with experimental observations showing that interfacial fracture rather occurs at incoherent interfaces. Finally, segregations effects are investigated.