

## MM 34: Topical Session: Fundamentals of Fracture - Fracture at the Atomistic Scale

Time: Wednesday 11:45–13:00

Location: H4

MM 34.1 Wed 11:45 H4

**Intergranular vacancies impact fracture** — ●DÖME TANGUY — Université de Lyon 1 France

Hydrogen has a strong binding to vacancies, which could lead to large vacancy concentrations. We study, by atomistic simulations, their possible impact on grain boundary fracture. Intergranular vacancy clusters are generated by Monte Carlo. The configurations are passed to MD and the critical loads for dislocation emission are compared to those for crack propagation. We report the minimum void size that triggers brittle propagation by "nano void" growth and discuss the crossover from intrinsic ductility to brittleness.

MM 34.2 Wed 12:00 H4

**hydrogen enhanced dislocation emission at a crack tip** — ●YU WANG<sup>1,2</sup>, DAMIEN CONNÉTABLE<sup>2</sup>, and DÖME TANGUY<sup>1</sup> — <sup>1</sup>Laboratoire de Physique de la Matière Condensée et Nanostructures, Université Claude Bernard Lyon 1, 43 Boulevard du 11 Novembre 1918, F 69622 Villeurbanne, France — <sup>2</sup>CIRIMAT, CNRS-UPS-INPT, ENSIACET 4 allée Emile Monso, BP 44362, F 31030 Toulouse, France

The influence of hydrogen on plasticity is an essential component of the modelling of H induced damage in structural metallic alloys. In this work, we study an idealized configuration where an atomistically sharp crack is loaded in mixed mode until a straight dislocation is emitted directly at the tip. It is shown, by Molecular Statics calculations using empirical EAM potentials, that the model proposed by Rice, which relates the critical stress intensity factor for emission ( $K_{IC}$ ) to the unstable stacking fault energy ( $\gamma_{us}$ ), is exact for dislocations moving along the crack plane (modes II or III dominate mode I), provided the influence of the mode I is taken into account in the  $\gamma_{us}$  calculation. The interest of combining Molecular Statics with the Rice model is that  $\gamma_{us}$  can be calculated on a system simple enough to be handled by ab initio methods. When dealing with hydrogen, on the contrary, there is no a priori knowledge how to introduce the H induced relaxations in the  $\gamma_{us}$  calculation, still preserving the relation between by  $\gamma_{us}$  and  $K_{IC}$  established by Rice. Therefore, Molecular Statics calculations with an empirical EAM potential for Al-H and Ni-H, on a large simulation box containing a crack,  $\gamma_{us}$  calculations with EAM potentials and ab initio calculations should be performed in parallel.

MM 34.3 Wed 12:15 H4

**Multiscale Modelling of Hydrogen Embrittlement in Zirconium Alloys** — ●JASSEL MAJEVADIA<sup>1</sup>, MARK WENMAN<sup>1</sup>, DANIEL BALINT<sup>1</sup>, ADRIAN SUTTON<sup>1</sup>, and ROMAN NAZAROV<sup>2</sup> — <sup>1</sup>Imperial College London, UK — <sup>2</sup>MPIE, Dusseldorf, Germany

Delayed Hydride Cracking (DHC) is a commonly occurring embrittlement phenomenon in zirconium alloy fuel cladding within Pressurized Water Reactors (PWRs). DHC is caused by the accumulation of hydrogen atoms taken up by the metal, and the formation of brittle hydrides in the vicinity of crack tips. The rate of crack growth is limited by the rate of hydrogen diffusion to the crack, which can be modelled by solving a stress driven diffusion equation that incorporates the elastic interaction between defects. This of interest in the present work.

The elastic interaction is calculated by combining defect forces determined through Density Functional Theory (DFT) simulations, and an exact solution for the anisotropic elastic field of an edge dislocation in Zr. making it possible to determine the interaction energy without the need to simulate directly a hydrogen atom in the presence of a crack or dislocation, which is computationally prohibitive with DFT.

The result of the elastic interaction energy calculations can be

utilised to determine the segregation of hydrogen to a crack tip for varying crack tip geometries, and in the presence of other crystal defects. This is done by implementing a diffusion equation for hydrogen within a discrete dislocation dynamics simulation. In the present work a model has been developed to demonstrate the effect of a single dislocation on hydrogen diffusion to create a Cottrell atmosphere.

MM 34.4 Wed 12:30 H4

**Multiscale Simulation of Brittle Fracture in Oxides and Semiconductors** — ●JAMES KERMODE — King's College London, Physics Department, London, WC2R 2LS, United Kingdom

Fracture is probably the most challenging 'multi-scale' problem: crack propagation is driven by the concentration of a long-range stress field at an atomically sharp crack tip. This creates a complex dynamical system with strongly coupled length scales. An accurate description of the chemical processes occurring in the small crack tip region is therefore essential, as is the inclusion of a much larger region in the model systems. Both these requirements can be met by combining a quantum mechanical (at the DFT level) description of the crack tip with a classical atomistic model that captures the long-range elastic behaviour of the surrounding crystal matrix, using a QM/MM (quantum mechanics/molecular mechanics) technique such as the 'Learn on the Fly' (LOTF) scheme. Here, we consider silicon and silica as prototypical semiconductor and oxide materials, respectively. The elastic and thermodynamic behaviour of silicon can be accurately described with simple interatomic potentials, while for silica a polarizable force field is required. Examples of the application of these techniques to fracture problems include low-speed dynamical fracture instabilities in silicon, interactions between moving cracks and material defects such as dislocations or impurities, very slow crack propagation via kink formation and migration, and chemically activated fracture, where cracks advance under the concerted action of stress and corrosion by chemical species such as oxygen or water.

MM 34.5 Wed 12:45 H4

**Brittle fracture of rutile TiO<sub>2</sub>: a first principles study** — ●BEATRIX ELSNER, WOLFGANG HECKEL, and STEFAN MÜLLER — Technische Universität Hamburg-Harburg, Institut für Keramische Hochleistungswerkstoffe, Denickestr. 15, D-21073 Hamburg

The potentiality of catastrophic failure poses a major challenge for the engineering application of brittle materials such as ceramics. Hence a fundamental understanding of the atomistic processes involved in brittle fracture is essential. Using density functional theory we have studied the failure of rutile titanium dioxide (TiO<sub>2</sub>) in loading mode I accounting for various cleavage plane orientations. For ideal brittle cleavage no surface relaxations are allowed and the universal binding energy relation (UBER) [1] can be applied to calculate the theoretical cleavage energy and corresponding strength. This yields the (110) and (100) planes as the equally most likely cleavage planes. Further, structural relaxations have been treated as they have a significant influence on the cleavage properties by lowering the cleavage energy. Unlike for metals [2] the onset of cleavage in TiO<sub>2</sub> cannot be easily derived from the energy separation curves and the relation between elasticity and cleavage will be discussed.

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[1] J. H. Rose, J. R. Smith, J. Ferrante, *Phys. Rev. B* **28**, 1835 (1983).

[2] P. Lazar, R. Podlucky, *Phys. Rev. B* **78**, 104114 (2008).