MM 31: Topical session (Symposium MM): Fundamentals of Fracture

Atomistic Aspects of Fracture II

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

Topical Talk MM 31.1 Wed 10:15 TC 006

Multiscale QM/MM Modelling of Materials Chemomechanics — •James Kermode — Warwick Centre for Predictive Modelling, School of Engineering, University of Warwick, Coventry, UK

Fracture is the dominant failure process underlying many materials reliability issues. At the same time, it remains one of the most challenging multi-scale modelling problems, requiring both an accurate description of the chemical processes occurring in the near tip region and the inclusion of a much larger region in the model systems. These requirements can be met simultaneously by combining a quantum mechanical 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) approach such as the 'Learn on the Fly* (LOTF) scheme [1]. I will review recent applications of this scheme to slow crack growth [2] and chemically activated fracture [3], and discuss a recent extension to the approach that uses the principle of virtual work with a modified nudged elastic band (NEB) algorithm to compute energy barriers for activated processes within the QM/MM framework [5]. The new method has been applied to compute lattice trapping barriers to brittle fracture in silicon as well and dislocation migration barriers in molybdenum and tungsten.

[1] G. Csányi et al., Phys. Rev. Lett. 93, 175503 (2004); [2] J. R. Kermode et al., Phys. Rev. Lett. 115, 135501 (2015); [3] A. Gleizer et al., Phys. Rev. Lett. 112, 115501 (2014); [5] T. Swinburne and J.R. Kermode, Phys. Rev. B 96, 144102 (2017)

MM 31.2 Wed 10:45 TC 006

The Brittle to Ductile Transition and the core structures of dislocations in silicon — •Jacques Rabier — Institut Pprime, DPMM, UPR 3346 CNRS-Université de Poitiers-ENSMA, BP30179, F-86962 Chasseneuil Futuroscope Cedex, France

It is now admitted that perfect shuffle dislocations control the plasticity of silicon in the high stress low temperature brittle domain and dissociated glide dislocations in the high temperature low stress domain [1]. The BDT appears then relevant to the transition between these two domains of plasticity. Unlike dissociated glide dislocations, core computations of perfect dislocations show that various core configurations can exist for a given dislocation. Some of these cores are sessile and differently from metals, these sessile dislocations cannot be mobilized under stress promoting the nucleation of crack [2]. Concurrently TEM experiments have shown that perfect dislocations nucleated in the brittle domain possess very efficient pinning points the density of which increases with temperature [2], [3]. Those pinning points appear to be intrinsic and relevant to some parts of sessile perfect dislocation cores. This induces a shut off of the perfect dislocations sources and a severe discontinuity in the apparent mobility of available dislocations close to the BDT, the consequences of which will be discussed.

[1] J Rabier, P Cordier, T Tondellier, J L Demenet, H Garem , Journal of Physics: Condensed Matter 12, 10059 (2000) [2] J. Rabier, L. Pizzagalli, J. L. Demenet, Elsevier B. V., 16, 47 (2010) [3] T. Okuno, H. Saka,, Journal of Materials Science, 48, 115 (2013)

MM 31.3 Wed 11:00 TC 006

Influence of large strains on the properties of dislocation cores in silicon: is a dislocation can initiate a crack? — •Laurent Pizzagalli, Julien Godet, and Sandrine Brochard — Institut Pprime, CNRS UPR 3346, Université de Poitiers, Poitiers, France

It is now well established that a usually brittle material like silicon can be plastically deformed at room temperature, if one considers low dimensional systems such as thin films, nanowires, nanopillars, or nanocubes. In these latter, due to the lack of bulk sources, the onset of plasticity usually occurs through the nucleation of dislocation from surfaces, and at large strains typically greater than 5%. The influence of these large strains on the properties of dislocation cores is usually overlooked and is currently unknown. We have investigated the properties of silicon 60° dislocation in these conditions, by performing atomistic calculations using several interatomic potentials, a tight-binding approach, and density functional theory. We found that the stability of the dislocation core is highly dependent on the imposed strain. In particular, it is revealed that a dislocation core could initiate a crack opening in conditions of bi-axial tension. Alternatively, we found that the formation of a localized disordered zone is favored in the case of bi-axial compression. These points constitute a possible explanation of the observed brittle-ductile transition as a function of size in nano-objects. Besides, this work also suggests that empirical interatomic potentials are not appropriate to describe dislocations in such conditions.

MM 31.4 Wed 11:15 TC 006

New theory for crack-tip dislocation emission and twinning in fcc metals — •Predrag Andric and William A. Curtin — Ecole Polytechnique Fédérale de Lausanne, Switzerland

Dislocation emission from a crack tip is a necessary precursor to crack blunting and toughening. Intrinsically ductile fcc metals under Mode I loading first emit a partial dislocation followed either by a trailing partial ("ductile" behavior) or a twinning partial ("quasi-brittle" behavior). The critical stress intensity factor K_{Ie} at which these processes occur is usually estimated by the Rice and Tadmor/Hai theories. Atomistic simulations show these models to be reasonable but not highly accurate, for predicting K_{Ie}. Analysis of the energy changes during nucleation reveals that the first and trailing partial emission are always accompanied by creation of a surface step, while twinning partial emission is not. Here, we present a new analysis in which first and trailing emission are controlled by a crack-tip instability due to the necessity of step formation. The absence of the step during twinning motivates another new model that accounts for the fact that twin nucleation does not occur directly at the crack tip. Both theories are quantitatively validated against molecular statics simulations across a wide set of fcc metals described with EAM potentials and excellent agreement is obtained. A twinning mode is also reported wherein the crack first advances by cleavage and then emits the twinning partial at the new crack tip.