MM 36: Topical Session (Symposium MM): Fundamentals of Fracture

Atomistic Aspects of Fracture III

Time: Wednesday 11:45–13:00 Location: TC 006

MM 36.1 Wed 11:45 TC 006

Cohesive stress heterogeneities and the transition from intrinsic ductility to brittleness — •Döme Tanguy — University Lyon 1, Villeurbanne, France

The influence of nanoscale cavities on the fracture of the Σ33{554}[110] symmetrical tilt grain boundary is studied by atomistic simulations. The crack crystallography is chosen such that dislocation emission is easy. A transition from a ductile behavior of the tip to a brittle one is obtained for a dense (coverage beyond 15% and inter-cavity spacing smaller than 4 nm) distribution of small cavities (sizes in between 1 and 2 nm). Nevertheless, the character of the crack is highly sensitive to the initial position of the tip and a mixture of ductile and brittle responses is found. A heterogeneous cohesive zone model, with parameters extracted from the simulations and enriched with a criterion for plasticity, can explain the simulations and reproduce the transition. Outside this range of small sizes and dense packing, dislocation half loops appear. They constitute, together with regions of low coverage/small cavities, efficient obstacles to brittle cracking. Furthermore, the generic character of the conclusions is evaluated by using the {554} single crystal to determine to which extent the results depend on the details of the core structure vs. the cavity distribution. Paper accepted in Phys. Rev. B.

MM 36.2 Wed 12:00 TC 006

Temperature Dependent Fracture Toughness of Defected Graphene — •Samaneh Nasiri, Debagyan Kalita, and Michael Zaiser — Friedrich-Alexander Universität Erlangen-Nürnberg, Department of Materials Science, Institute for Materials Simulation WW8 and Cluster of Excellence EAM/FUMIN Dr.-Mack-Strasse 77, 90762 Fürth, Germany

It is well known that sp* bonded carbon nanoparticles, in particular Graphene and Carbon Nanotubes, possess excellent mechanical properties in terms of in-plane elastic modulus and rupture strength. It is therefore an obvious question whether these properties can be influenced by defects. The present work investigates crack nucleation and crack propagation in defected graphene sheets over a wide range of temperatures. We consider the fracture behavior of graphene containing localized defects (vacancies) and/or extended defects (cracks) using atomistic (molecular dynamics) simulation. Fracture strength is shown to obey a Bazant-type size effect law where the internal length (process zone size) is of the order of the atomic spacing. The fracture toughness is also calculated in terms of the critical stress intensity factor for various temperatures from zero to as high as 3200 K. Results indicate a transition towards a different failure behavior and crack propagation pattern at temperatures above 2000K which may be interpreted in terms of a sub-nanometer scale brittle-to-ductile transition.

Keywords: graphene, fracture, temperature, crack, toughness, brittle-ductile transition

MM 36.3 Wed 12:15 TC 006

T-stress and the brittle-ductile behavior of edge cracks in 3D iron crystals — Anna Machová, •Radek Kolman, Alena Uhnáková, and Petr Hora — Institute of Thermomechanics, v.v.i., CAS, Dolejskova 5, 18200 Prague 8, Czech Republic

According to continuum treatment, the sign of T-stress in SEN specimens loaded uni-axially in mode I depends on boundary conditions and sample geometry. Since the sign of the T-stress can change theoretically brittle vs. ductile behavior of cracks, we verified recently the continuum predictions via molecular dynamic simulations (MD) in 3D bcc iron atomistic samples of SEN type. Crack orientation is (-110)[110] (crack plane/crack front), the axis of potential crack extension corresponds to [001] direction.

Under boundary conditions corresponding to constant stress at the borders the T-stress sign is negative for a short edge. For a relatively long crack it is positive. At higher level of linear loading, dislocation emission on <111>{112} slip systems was detected at the short crack with negative T-stress, while cleavage or brittle fracture was detected at the long crack with positive T-stress under relatively slow loading rates.

Behavior of relatively long cracks has been studied under constant displacement conditions, where negative T-stress is predicted. MD stress calculations confirm the change of the T-stress sign with the change of boundary conditions. Under higher loading, dislocation emission on <111>{112} slip systems and crack blunting were detected.

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MM 36.4 Wed 12:30 TC 006

Modelling Chemomechanical Materials Failure Processes in SiC and Diamond — •Punit Patel and James Kermode — University of Warwick, United Kingdom

Atomistic simulations of crack propagation are key to understanding the fracture behaviour of materials. Cracks involve strong coupling across the scales, with bond breaking on the quantum scale driven by long range stress fields. Current QM methods are limited to simulation sizes too small to accurately describe fracture dynamics and improved QM/MM methods are able to adequately capture elastic effects [1]. However these methods are still heavily limited temporally and to coarse grain into the continuum scale while maintaining the overall fracture dynamics an expanded multiscale approach is required.

Applications in covalently bonded single crystals to complex alloys are underway. Screened classical potentials [2] predict a brittle response in both silicon carbide (SiC) and diamond, giving confidence in their applicability. DFT SiC surface energy calculations produced predictions in good agreement with experiment [3]. Extension of the multiscale approach for fracture includes a novel approach in correcting for finite domain boundary conditions in order to compute energy barriers for crack extension bridging DFT and long time scale MD.

[1] N. Bernstein et al., Rep. Prog. Phys. 72, 026501 (2009).
[2] L. Pastewka et al., Phys. Rev. B. 87, 205410 (2013).
[3] G. Sernicola et al., Nat. Commun. 8, 108 (2017)

MM 36.5 Wed 12:45 TC 006

Atomistic-based fracture criteria for continuum models — Johannes Möller[1,3], Hamad ul-Hassan[2], Erik Bitzek[1], Alexander Hartmaier[2], and •Rebecca Janisch[2] — [1]Friedrich-Alexander Universität Erlangen-Nürnberg — [2]ICAMS, Ruhr-Universität Bochum — [3]Fraunhofer Institut für Werkstoffmechanik, Freiburg

Continuum mechanics provides an efficient way to model fracture at the engineering scale, based on stresses, stress intensity factors, and energy release rates. Additionally, material-specific information and failure criteria are required to describe fracture at this scale. At the atomic scale, in contrast, the breaking of atomic bonds is caused by critical forces acting on individual atoms. Here, we present a systematic, mesh-independent approach that directly connects the interatomic forces to stress-based failure criteria for finite element implementations of continuum models. We base our approach on a detailed analysis of the forces acting between the atoms in front of a crack tip, as well as between two semi-infinite half-crystals, the latter being the common approach, e.g., for ab-initio density functional theory calculations of cohesive properties. The analysis shows, that the interatomic forces at a crack tip can be directly related to the restoring tractions between the two planar surfaces. This allows for an unambiguous scaling of the critical stresses and displacements, from GPa / Å on the atomic level, to the order of hundreds of MPa and nm on the mesoscale. The implementation in a finite element scheme will be demonstrated.