Atomistic Simulations of Fracture and Crack-Microstructure Interactions in BCC Metals

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The resistance to crack propagation is undoubtedly one of the most important properties of structural materials. Whether a stressed component fractures by brittle cleavage or by ductile rupture is determined by the competition between bond-breaking at the crack tip and plastic deformation in the vicinity of the crack. Which of these processes dominates at a given temperature and strain rate depends on the nature of the chemical bond between the atoms as well as on the microstructure of the material. While meso- and continuum-scale methods can be used to model the elastic loading of the crack tip and the plastic dissipation in the process zone, only atomistic simulation methods can be used to study the direct interactions between cracks and constituents of the microstructure (e.g., dislocations, grain boundaries, particles or voids) or the nucleation of dislocations at the crack front[1]. However, up-to-date most atomistic fracture simulations use idealized setups with perfectly straight crack-fronts in quasi-2D geometries. Only few simulations address the full complexity of 3D crack - microstructure interactions, including curved crack fronts and dislocations on oblique slip systems. Here we present our recent work on large-scale atomistic fracture simulations using EAM-type potentials for α-Iron and other BCC metals, focusing on often neglected 3D aspects.

The first part will be devoted to a tutorial-style overview of different approaches to perform atomistic fracture simulations, explaining the methodological background and challenges as well as providing best practices regarding the selection of interatomic potentials[2], simulation setups and boundary conditions. We then compare the results of straight crack fronts in quasi-2D set-ups with curved crack fronts in 3D set-ups[3]. General aspects relevant for crack-microstructure interactions in BCC metals will be discussed using exemplary simulations of cracks interacting with pre-existing dislocations, voids and precipitates in 3D. Finally, quasi-2D grain boundary fracture simulations[4] will be compared to recent large-scale simulations on penny-shaped grain boundary cracks. All these results demonstrate the importance of 3D models to study crack nuclei and crack-obstacle interactions and the inability of 2D models with straight crack fronts to predict the behavior of curved crack fronts.

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