Predicting Fracture Toughness ab-initio: Discrete Dislocation Plasticity Informed by Quantum-accurate Atomistic

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Predicting fracture toughness of bcc transition metals as a function of temperature is challenging since multiple mechanisms are activated, such as dislocation emission from crack-tip, debonding of crack-tip atoms, and interaction between crack and pre-existing dislocations. To capture the fundamental mechanisms that originate at the atomistic scale, extensive molecular dynamics (MD) modelling[1, 2] has attempted to reveal the crack propagation mechanisms which is important for predicting fracture toughness. However, no pre-existing dislocations are included in those atomistic models due to their expensive computational cost. This results in a predicted fracture toughness that is orders of magnitude lower than the experimental measurements[3]. A multi-scale approach is therefore required to enable the prediction of fracture toughness, whereby pre-existing dislocations are explicitly taken into account.

Here, to bridge the scales from the atomic to the micro-scale, we employ discrete dislocation plasticity (DDP), which is informed by a quantum-accurate atomistic model[3]. The atomistic model is validated on a broad range of properties that are crucial to simulate dislocation plasticity and fracture (elastic constants, surface energy, stacking fault energy etc.) The dislocation emission process from atomistic is analysed to obtain physical parameters as inputs for DDP. Based on the atomistic model, nudged elastic band calculations are performed to obtain the activation barrier for a number of dislocations, including screw, $71\mathrm{deg}$ mixed, and edge type. A mixed mobility law is established subsequently. A cohesive zone model is used to describe the crack propagation. The dislocation emission process is incorporated by including Frank-Read sources near the tip. We implement corresponding changes in a 2D discrete dislocation framework [4].

To investigate the influence of pre-existing dislocations, we generate a series of initial dislocation distribution by loading and unloading of a rectangle specimen. The competition among crack propagation, dislocation emission from crack-tip, and thermally activated dislocation in the bulk is analysed. Next, the crack-blunting introduced by dislocation emission from crack-tip are studied by starting with different crack-tip geometry. The predicted fracture toughness is compared to experiments. Our work is a systematic approach to model fracture ab-initio up to the micro-scale, showing the necessity of a multi-scale approach for predicting fracture toughness.

References

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