

ATOMISTIC SIMULATION OF FRACTURE INITIATION AT SHARP NOTCHES IN SILICON

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ABSTRACT

We have previously developed a theory to predict fracture initiation at near atomistically sharp corners in single crystal silicon. The theory suggests that fracture will initiate from a sharp corner with no pre-existing crack when the stress intensity associated with the singular elastic field reaches a critical value. The theory is based on ideas analogous to classical small scale yielding in linear elastic fracture mechanics, and has been validated experimentally. In this talk we study issues regarding the small scale yielding type arguments using direct atomistic simulations using the modified embedded atom method (MEAM) potential. We study the departure from linear elasticity near the tip of atomistically sharp corners (such as those that occur naturally by etching in KOH) as the fracture load is approached. We attempt to draw conclusions regarding the nature of the atomic separation process and its control by the stress intensity for different local geometries (corner angles). The atomistic simulations predict the experimentally observed sensitivity to cleavage of $\{111\}$ and $\{110\}$ planes, including an interesting zig-zag crack propagation along alternating families of $\{111\}$ and $\{-111\}$ planes.