Atomistic Modeling of Materials Failure

Christian Thaulow[1]

[1] Department of Engineering Design and Materials, The Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

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Whether a material is ductile or brittle depends on the competition of intrinsic material parameters (such as the energy required creating new surfaces versus the energy required to initiate shearing of the lattice to form and move a dislocation). The type of mechanical failure response will be controlled by the temperature and deformation rate. Experimental studies of single crystal silicon with pre-cracks have shown that at temperatures below about 850K the material tends to be extremely brittle, while it exhibits ductile behavior above this temperature. Several explanations have been proposed; however, thus far no direct atomistic level understanding exists about the underlying process that leads to BDT in silicon. This progress has been hindered partly due to lack of atomistic models that enable the simulation of sufficiently large systems to accurately describe the fracture process.

Describing bond breaking processes in silicon has required quantum mechanical (QM) methods to properly describe the complex electronic rearrangements that determine the barriers and hence rates. However, quantum mechanics calculations for large system sizes that would be required to describe the complex details of bond rearrangements under large stresses are currently impractical. In this investigation we apply an alternative approach; the first principles based ReaxFF reactive force field, which retains nearly the accuracy of QM, even for bond breaking events. The ReaxFF parameters are determined by fitting QM-data on silicon and allow us to directly simulate BDT.

By solely raising the temperature in a series of computational experiments with otherwise identical boundary conditions, we observe a sudden change from brittle to ductile behavior between 880 K and 890 K, drastically changing the material in a very narrow ≈10 K temperature regime. Our studies elucidate a cascade of atomic mechanism that control the occurrence of the BDT. We find that at elevated temperatures, the formation of a small amorphous region at an atomically sharp crack tip creates a cleavage ledge at the crack tip, inducing local mode II (shear) stresses at the crack tip, which in turns leads to dislocation emission. Our results address provide a fundamental understanding of the link between stress the crack tip geometry, associated structural changes under temperature variations, and the overall mechanical behavior of a solid. Our simulations provides important insight into the atomistic-level mechanism of the brittle-to-ductile transition in silicon, with relevance for other materials that undergo BDT.