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Multiscale Simulations of High-Temperature Fracture in Silicon

NOAM BERNSTEIN, Naval Research Lab — We simulate the effects of temperature on the dynamic fracture process in silicon. We use a dynamically coupled method that combines tight-binding at the crack tip with empirical potentials far from the tip in a molecular dynamics (MD) simulation.[1] This method has been shown to give brittle fracture at low temperatures, in agreement with experiment.[1]. Here we present simulations of fracture at high temperatures, about 1000 K. These simulations are carried out in a strip geometry, and are relatively long and well equilibrated. There is no evidence that the velocity gap closes at these temperatures, at least not on the MD time scale. Fluctuations manifest themselves in the spontaneous nucleation of defects at the crack tip. We discuss the nature and evolution of the defects, and their possible relation to the sharp brittle-to-ductile transition observed in silicon.

[1] N. Bernstein and D. Hess, MRS Proc. vol. 653 (2001); – Phys. Rev. Lett. vol. 91 (2003).

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