419g Feature Activated Molecular Dynamics Simulation of Void Cavitation in Crystalline Silicon under Dynamic Tension

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Molecular dynamics simulation is ideally suited for the study of complex dynamical atomistic processes in solids, ranging from defect diffusion and aggregation to crack propagation and fracture. However, the computational limitations of the method has led to much interest aimed at developing approaches to extend the accessible length and time scales. Here we present a recently developed simulation method based on molecular dynamics (Feature Activated Molecular Dynamics, or FAMD [1]), which we apply to the study of void cavitation under dynamic hydrostatic tension in crystalline silicon.

In the FAMD simulations presented here, only the region immediately surrounding the cavity is simulated with MD ("active" regions), while regions further away ("static" regions) are periodically subjected to partial static relaxation under boundary conditions imposed by the active regions. As the cavity expands and changes shape, the active region automatically adapts to ensure that it is fully contained. We show that the algorithm provides a good representation of the cavitation dynamics, while offering substantial advantages over standard MD. The cavitation process is studied as a function of temperature, strain rate, and initial void morphology.

[1] M. Prasad and T. Sinno, J. Chem. Phys., 121, 8699 (2004).