559i Isostress Molecular-Dynamics Analysis of the Structural Response of Cubic Metallic Crystals to Hydrostatic Tension

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Understanding large-strain mechanical deformation and failure of crystalline solids requires analyses of elastic stability in order to determine the crystal's mechanical strength. At given temperature, the structural response of a crystal to applied mechanical loading according to a certain loading mode becomes unstable beyond a critical stress level. This might lead to fracture of the crystal. Determining the onset of elastic instability and analyzing the structural response of the crystalline solid beyond the instability onset is a topic of major interest in the mechanics of crystalline materials.

In this presentation, we focus on the structural response of face-centered cubic (fcc) crystals subjected to hydrostatic tension. We report results of systematic analyses of the elastic stability of such crystals based on isostress molecular-dynamics (MD) simulations according to the Lagrangian formulation of Parrinello and Rahman. In the simulations, interatomic interactions are expressed by classical force fields that have been fitted to experimental elastic moduli of metals and yield large-strain nonlinear elastic behavior in excellent qualitative agreement with more sophisticated atomistic models and with experiment. We examine in detail geometric, mechanical, energetic, and kinetic characteristics of elastic instabilities that cause failure of the crystal. In addition to the detailed monitoring of atomic-scale dynamics, we use canonical strain fluctuation formulae to compute elastic moduli as functions of temperature and stress; these moduli are used in rigorously derived criteria for the assessment of crystal elastic stability. The simulation results for the structural response of crystals to loading beyond the instability onset are quite general, regardless of the atomic model used to describe interatomic interactions in the metallic crystals under consideration. This is demonstrated by systematically comparing lattice-statics calculations of crystal structural response based on simple descriptions of interatomic interactions in metals using pair potentials with the same calculations using more realistic descriptions according to the embedded-atom method.

Results are presented for the structural response to hydrostatic tension of several model crystals that have an fcc lattice structure at equilibrium. In all cases, it is demonstrated that the observed instabilities are thermally activated and associated with a vanishing or diminishing bulk modulus and that the instability triggers the fracture of the fcc crystal. In addition, the temperature dependence is calculated of the critical stress for the instability onset and of the thermal activation enthalpy barrier that should be overcome for the fracture process to take place beyond the instability onset. Specifically, the critical stress and the activation enthalpy are monotonically decreasing and monotonically increasing functions of temperature, respectively, and the enthalpy barrier vanishes completely as the temperature is lowered to absolute zero. The MD simulation results at low temperature are in excellent agreement with the predictions of the stability criteria according to “static” elastic stability theory.