177b Elastic Instability of Cubic Crystals under High Hydrostatic Tension: Atomic Pattern Formation Leading to Structural Transformation or Failure

Hadrian Djohari, Frederick Milstein, and Dimitrios Maroudas

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 following a certain loading mode becomes unstable beyond a critical stress level. In spite of numerous studies aiming to evaluate the theoretical strength of crystals, identifying and analyzing the prevailing atomic mechanisms of a crystal's structural response beyond the onset of stress-induced instability remains a major challenge in materials mechanics.

In this presentation, we report results of systematic elastic stability analyses in metallic 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 instabilities in crystals under stress, placing special emphasis on the atomic pattern formation characteristics in the crystals' structural response to loading at and beyond the onset of elastic instability. 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 results of our simulations are quite general for the structural response of crystals to loading beyond the critical state that marks the onset of elastic instability, 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 several specific interesting cases of structural transformation in cubic crystals under hydrostatic tension. Our analysis emphasizes bifurcations in the crystal structural response that is exhibited when the applied hydrostatic load and/or the temperature are varied, as well as the atomic pattern formation characteristics beyond the instability onset. The atomic-scale analysis reveals the structural transformation mechanism and elucidates the atomic pattern formation dynamics that may lead to either structural transformation or crystal failure beyond the elastic instability. The structural transformations that will be discussed include a case where a simple cubic lattice transforms to a hexagonal close packed (hcp) structure at very low temperatureand a body-centered cubic (bcc) transforms to an hcp or a face-centered cubic (fcc) structure depending on the thermomechanical conditions of loading. In all cases, the observed instabilities are found to be associated with vanishing or diminishing elastic moduli and the simulation results are discussed in the context of the theoretical stability criteria.