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Theoretical Analysis of Stress-Induced Structural Response of Cubic Crystals Beyond the Onset of Elastic Instability HADRIAN DJOHARI, Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003-3110, JIANHUA ZHAO, Departments of Materials and Mechanical Engineering, University of California, Santa Barbara, CA 93106, FREDERICK MILSTEIN, Departments of Materials and Mechanical Engineering, University of California, Santa Barbara, CA 93106, DIMITRIOS MAROUDAS, Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003-3110 — Determining the mechanical strength of crystalline materials requires elastic stability analyses for fundamental understanding of crystal large-strain deformation and failure. In this presentation, we report results of systematic elastic stability analyses in metallic crystals based on isostress molecular-dynamics simulations that capture in detail the mechanical, geometric, and kinetic aspects of stress-induced instabilities. Our analysis emphasizes bifurcations in the crystal structural response exhibited as the applied load is varied and atomic pattern formation characteristics beyond the instability onset. Results are presented for various cases of structural evolution under hydrostatic and uniaxial [100] and [111] loading for model crystals that have an fcc structure at equilibrium. The corresponding structural responses range from inhomogeneous structural transitions to fracture through decohesion and voiding. The observed instabilities are thermally activated and associated with vanishing or diminishing combinations of elastic moduli.

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