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Elastic Stability Analysis of the Structural Response of Cubic Crystals to Hydrostatic Loading HADRIAN DJOHARI, Department of Chemical Engineering, University of Massachusetts, Amherst, MA 01003-3110, 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 —
We report results of systematic elastic stability analyses in metallic crystals based on isobaric molecular-dynamics simulations that capture the mechanical, geometric, and kinetic aspects of instabilities induced under hydrostatic loading. Our analysis emphasizes bifurcations in the crystal structural response 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 loading for model crystals that have a cubic lattice structure at equilibrium, including crystals with structural heterogeneities such as internal nanovoids and free surfaces. 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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