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Strain Relaxation through Structural Phase Transition in Ultra-thin Films of FCC Metals KEDARNATH KOLLURI, M. RAUF GUNGOR, DIMITRIOS MAROUDAS, University of Massachusetts, Amherst — We report a computational analysis of atomistic mechanisms of relaxation of biaxially applied tensile strain over a broad range of strain levels, ε, in freestanding ultra-thin Cu films based on isothermal-isostrain large-scale molecular-dynamics simulations. Our analysis reveals that for $\varepsilon < 10\%$, plastic deformation occurs through ductile void growth and dislocation nucleation and glide from the thin-film surfaces. For $\varepsilon \geq 10\%$, strain relaxation is dominated by the nucleation of a high density of dislocations at the film's surface, leading to a martensitic transformation of the thin film from an fcc to a hcp lattice structure. The hcp phase nucleates at the surface of the thin film and propagates into the film due to the glide of dislocations; in this process, the relative atomic slips have magnitudes identical to those observed in Bain transformations. Furthermore, mechanical analysis according to generalized stability criteria shows that the observed phase transition is consistent with the onset of a shearing instability of the thin film.

Kedarnath Kolluri
University of Massachusetts, Amherst

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