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Computational Study of Atomistic Strain Relaxation Mechanisms in Biaxially Strained Ultra-Thin Metallic Films M. RAUF GUNGOR, University of Massachusetts, Amherst, DIMITRIOS MAROUDAS, University of Massachusetts, Amherst — Understanding the mechanical response under certain loading conditions of nanometer-scale-thick metallic films is fundamentally and technologically important. In this presentation, we report a comprehensive computational analysis on the atomistic mechanisms of strain relaxation under a wide range of applied biaxial tensile strain in free-standing ultra-thin Cu films based on multimillion-atom molecular-dynamics simulations. Our analysis reveals that after an elastic response at low strain (< 2%), plastic deformation occurs accompanied by dislocation emission from the void surface, void surface morphological transition, dislocation jogging, vacancy generation and migration along dislocation cores, as well as formation and propagation of threading dislocation loops from the film's surfaces. At higher (> 6%) strain levels, a transition to a new plastic deformation regime gives rise to a practically uniform distribution of dislocations in the metallic thin film. Under such conditions, dislocations are emitted from the thin film's surfaces and inhibit void growth due to their interactions with the dislocations emitted from the void surface and the resulting pinning of the latter defects.

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