Atomistic Calculations for the Mechanical Instability of Nanoscale Structures

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We investigate the instability behaviors of FCC metal single structures and nanowires under uniaxial tensile and compressive loadings by conducting molecular dynamics and static simulations. In terms of the stiffness moduli of a single metal crystal, we compare our simulation results with the Hill and Milstein's instability condition. Under tensile loading for a bulk system, the symmetry of the system changes from tetragonal to orthorhombic at the critical strain which is consistent with the prediction of the Hill and Milstein's instability condition. However, the phase transformation occurs later as the thickness of metal nanowires decreases compared to the bulk case, due to different surface effects. In addition, we find highly anisotropic deformations when a uniaxial tensile loading is applied to metal nanoplates.

Keywords: Instability, Atomic Simulation, Nanowire, Nanoplates