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Density Functional Investigation of Surface Stress-Induced Phase Transformations in FCC Metallic Nanowires MICHAEL HAFTEL, Naval Research Laboratory, KEN GALL, Georgia Institute of Technology — We use density functional theory (DFT) to study the relaxation of narrow Cu, Ni, Au, Pt and Ag nanowires originally oriented in the <001> direction with a FCC structure. For a small enough diameter (D<2 nm) each nanowire, under the compressive influence of its own surface stress, spontaneously relaxes to either a <110> orientation (Cu, Ni, Ag) or to a BCT <001> (Au, Pt) orientation, both of which are characterized by a compression of the wire axis of at least 30%. To analyze the stability of BCT structures, we calculate the elastic constants for the BCT phases of these metals under bulk, slab, and nanowire conditions. We find that the surface contribution to the elastic constant for shear, C_{66}, helps stabilize the BCT phase in Au which would otherwise be unstable under bulk conditions. A large stabilization contribution from the surface also occurs in Ni and Cu, but not enough to overcome the shear instability in the bulk, and these nanowires do not transform to BCT. We discuss the implications of these results on the superelastic shape-memory effect for FCC metals.

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