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Martensitic phase transitions in metallic nanowires MICHAEL HAFTEL, Naval Research Laboratory, KENNETH GALL, University of Colorado, JIANKUAI DIAO, Washington University, NOAM BERNSTEIN, MICHAEL MEHL, Naval Research Laboratory — We use the NRL tight binding method (TB) and modified embedded atom method (MEAM) to investigate the spontaneous phase transition from fcc to bct for Au nanowires oriented in the (001) direction. Employing density functional theory (DFT) calculations of the energy of bulk Au under uniaxial strain along the Bain path, we find that bulk Au has a minimum along this path for a bct structure, which, under uniaxial stress of greater than $\sim$2 GPa, would become energetically favorable to the fcc structure. This state, however, is unstable with respect to shear deformation. The TB method predicts the same behavior. TB simulations of Au nanowires smaller than 2.0 nm diameter, however, indicate that that these nanowires will spontaneously relax from an original fcc structure to a bct structure even at 0 K and zero external pressure. The driving force for the transition is the surface stress along the outer boundary of the nanowire, which provides the necessary 2 GPa of total stress to effect the phase transition. Furthermore, the surface stress stabilizes the bct structure with respect to shear. Its stability is verified by TB simulated annealing and large-scale MEAM simulated annealing simulations. We will also discuss a TB model for the shape-memory NiTi alloy and its use in nanowire simulations.

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