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Absence of metastable states in strained monoatomic cubic crystals. AARÓN AGUAYO, Facultad de Matemáticas, Universidad Autónoma de Yucatán, México., MICHAEL L. MEHL, L.L. BOYER, Naval Research Laboratory, Washington, DC 20375-5345, USA, ROMEO DE COSS, Department of Applied Physics, Cinvestav-Mérida, México. — The Bain path distortion of a metal with an fcc (bcc) ground state toward the bcc (fcc) structure initially requires an increase in energy, but at some point along the Bain path the energy will again decrease until a local minimum is reached. We have studied the tetragonal distortion (Bain path) of monoatomic cubic crystals, using a combination of parametrized tight-binding and first-principles linearized augmented plane wave calculations. We show that this local minimum is unstable with respect to an elastic distortion, except in the rare case that the minimum is at the bcc (fcc) point on the Bain path. This shows that body-centered-tetragonal phases of these materials, which have been seen in epitaxially grown thin films, must be stabilized by the substrate and cannot be free-standing films. This work was partially supported by Consejo Nacional de Ciencia y Tecnología (CONACYT, México) under Grant No. 43830-F.

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