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Atomistic modeling of thermodynamic equilibrium of plutonium TONGSIK LEE, STEVE VALONE, Los Alamos National Laboratory, MIKE BASKES, Los Alamos National Laboratory and University of California, San Diego, SHAO-PING CHEN, Los Alamos National Laboratory, ANDREW LAWSON, Retired — Plutonium metal has complex thermodynamic properties. Among its six allotropes at ambient pressure, the fcc delta-phase exhibits a wide range of anomalous behavior: extraordinarily high elastic anisotropy, largest atomic volume despite the close-packed structure, negative thermal expansion, strong elastic softening at elevated temperature, and extreme sensitivity to dilute alloying. An accurate description of these thermodynamic properties goes far beyond the current capability of first-principle calculations. An elaborate modeling strategy at the atomic level is hence an urgent need. We propose a novel atomistic scheme to model elemental plutonium, in particular, to reproduce the anomalous characteristics of the delta-phase. A modified embedded atom method potential is fitted to two energy-volume curves that represent the distinct electronic states of plutonium in order to embody the mechanism of the two-state model of Weiss, in line with the insight originally proposed by Lawson et al. [Philos. Mag. 86, 2713 (2006)]. By the use of various techniques in Monte Carlo simulations, we are able to provide a unified perspective of diverse phenomenological aspects among thermal expansion, elasticity, and phase stability.

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