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Density-Functional Calculations of α-Pu-Ga (Al) Alloys ALEXANDER LANDA, PER SODERLIND, Lawrence Livermore National Laboratory, Livermore, CA 94550, LEVENTE VITOS, Royal Institute of Technology, Stockholm, SE-10044, Sweden — At atmospheric pressure plutonium metal exhibits six crystal structures. The least dense phase (δ-Pu) has a 25% larger volume than the ground-state (α-Pu) phase and is thermodynamically stable at temperatures between 593 and 736 K. In order to extend the stability of δ-Pu to ambient temperatures, plutonium is alloyed with a small amount of so-called 'δ-stabilizers', for example, Ga or Al. The α-phase has no equilibrium solubility with any of these δ-stabilizers but upon cooling of the δ-Pu-Ga (Al) alloys, under certain conditions, Ga (Al) atoms can be trapped in the α-lattice causing an expansion. First-principles methods are employed to study the ground-state atomic volumes of α-Pu-Ga (Al) alloys. It was shown that a random distribution of Ga (Al) atoms in the monoclinic lattice of α-Pu results in a maximum expansion of this lattice. Any kind of ordering of Ga (Al) on the monoclinic lattice results in shrinking of the lattice constant while the ordered α_8-(Pu-Ga (Al)) configuration yields the smallest lattice constant which is very close to that of pure α-Pu. In addition, energetics of the ordered and disordered configurations is discussed. This work was performed under the auspices of the U.S. Department of Energy by the University of California Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

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