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Dynamical stability of plutonium alloys MARC TORRENT, BORIS DORADO, JORDAN BIEDER, CEA, DAM, DIF (Atomic and Alternative energies Commission, France) — Plutonium sits at the center of the actinide series and marks the transition between localization and delocalization of the $5f$ electrons. From a metallurgical standpoint, the monoclinic α phase (stable at low T) is brittle, not suitable for engineering applications, as opposed to the ductile fcc δ phase (stable at 580K). The $\delta - \alpha$ transition can be avoided by alloying δ-Pu with "deltagen" elements. There is a wide unexplored area for Pu when it comes to lattice dynamics. Due to the changes in the composition, the dynamical stability of is constantly challenged. Displ. cascades are created in the material, which in turn produce numerous of point defects. Therefore, the accumulation of defects preclude a thermodynamic equilibrium. Given the importance for engineering applications, it is crucial that we understand the mechanisms that lead to stabilization with respect to the alloy composition. We use first-principles calculations to provide evidence of the effect of defects/impurities (C, O, Al, Fe, Ni, Ga, Ce, U, Am) on the dynamical stability of δ-Pu. We show that this phase is dynamically unstable at low T and that it depends on the $5f$ orbital occupancies. We investigate how defects affect the stability by comparing the phonon DoS.

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