

Abstract Submitted
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Phonon mechanisms for structural phase transitions in Pu AVADH SAXENA, TURAB LOOKMAN, R.C. ALBERS, Los Alamos National Laboratory, CONDENSED MATTER THEORY TEAM — As a function of temperature, pressure and alloying (Ga or Al) plutonium undergoes a series of structural transitions. Based on crystallography and symmetry we identify possible phonon mechanisms for various phase transitions. Coupling of shuffle modes corresponding to the specific phonons (primary order parameter) to the relevant strain tensor components (secondary order parameter) we develop Ginzburg-Landau free energies for some of the important structural transitions such as $\delta \rightarrow \alpha$ (FCC to simple monoclinic), $\delta \rightarrow \beta$ (FCC to side centered monoclinic) and $\beta \rightarrow \alpha$ (side centered monoclinic to simple monoclinic). We use these free energies to explore certain parts of the Pu phase diagram and relate to experimental structural and thermodynamic data such as specific heat and thermal expansion for the cases available. We also enumerate the orientational relationships between parent and product phases in these transitions.

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