

Structural and Thermophysical Properties of Pu Intermetallics

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Plutonium is arguably the most complex element in the periodic table. It sits near the middle of the actinide series, precisely in between where the 5f electrons are involved in bonding, as in the transition metals and light actinides (Th-Np), or are localized close to atomic core and do not contribute to bonding, as occurs in the lanthanides or heavy actinides (Am-Lr). This itinerant to localized crossover can be observed in the trends of the Wigner-Seitz radii of the transition metals, lanthanides, and actinides, where plutonium, particularly its cubic δ -Pu phase, lies in between localized and itinerant behavior. The near degeneracy of these two bonding configurations leads to a variety of unusual behavior, including six different allotropic phases, mechanical properties ranging from extremely brittle to ductile, and the largest Sommerfeld coefficient of all the elements. These interesting properties are derived from the 5f electrons of plutonium. An understanding of the subtle changes in electronic structure at this localized/itinerant crossover of Pu's 5f electrons is still lacking. Experiments capable of revealing the electronic structure, such as angle-resolved photoemission or de Haas van Alphen measurements, have not been possible because single crystalline samples of Pu are not easily synthesized. However, single crystals of plutonium compounds, which exhibit a range of behavior from localization to itinerancy of Pu's 5f electrons and are suitable for these measurements, may shed light on the physics near the localization/delocalization transition.

Pu₆M (M = transition metal) compounds crystallize in the U₆Mn-type with the tetragonal space group *I4/mcm* (No. 140). The building blocks that compose the Pu₆M structure are Pu1 distorted octahedral units and Pu2 face-shared square antiprisms that have transition metal atoms preferentially occupying their centers. The Wyckoff positions of the Pu1, Pu2, and M atoms are 8h, 16k, and 4a, respectively. The Pu₆M compounds can be easily prepared by arc melting. The rich structural chemistry, microstructure, and thermophysical properties of these compounds are exemplified through a suite of techniques including X-ray diffraction, heat capacity, and electron microscopy.