Hysteretic Phase Transition Predicted in Indium-Plutonium Alloy

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Elemental plutonium (Pu) assumes more crystal structures than other elements, plausibly due to bonding f electrons becoming non-bonding. Complex geometries hamper understanding of the transition in Pu, but calculations predict this transition in a system with simpler geometry: alternating layers of plutonium and lead (Pb).[1,2] Here the transition occurs via a pairing-up of planes within Pu layers.

Replacing the Pb layers with indium (In) layers leads to analogous results. In particular, the transition appears in the limit of monatomic thin layers.[3] This system corresponds to the experimentally observed θ-InPu phase of the alloy, but with the crystal symmetry broken either (i) by the pairing of the Pu atoms, or (ii) by a trigonal distortion. The calculations predict that these broken-symmetry structures stabilize at low temperatures, where uniaxial strain induces the transition between them. The transition shows hysteresis in the character of the electronic state, in the Pu-Pu bond lengths, and in the density.

[1] Sven P. Rudin, Phys. Rev. Lett. **98**, 116401 (2007).

[2] Sven P. Rudin, Phys. Rev. B **76**, 195424 (2007).

[3] Sven P. Rudin, Phys. Rev. B **77**, 172104 (2008).