Origin of β-cerium investigated with ab initio calculations of stacking fault energies

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At zero pressure the element cerium shows a metastable ($t_{1/2} \sim 40$ years) double hexagonal close-packed β-phase that is positioned between two cubic phases, γ and α. With modest pressure the β-phase can be suppressed, and a volume contraction (17%) occurs between α and γ phases as temperature is varied. This phenomena has been linked to subtle alterations in the $4f$ band. In order to rationalize the presence of the metastable β-phase, and its position in the phase diagram, we have computed stacking fault formation energies of the cubic phases of cerium. It is found that there is a large difference in the stacking fault energies between the α and γ-phase. The β-phase energy is nearly degenerate with the γ-phase, and can be seen as a dislocation reservoir that appears to be necessary to accommodate the large strains generated during the α-γ transition. Such a degeneracy explains long standing third law calorimetry results, and dislocation dynamics the pressure and temperature hysteretic effects.

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