Materials Science in Semiconductor Processing, vol. 16(6), 2013, pages 1508-1516

Structural, elastic, electronic and thermodynamic properties of the filled skutterudite CeOs4Sb12 determined by density functional theory

Abstract

Structural, elastic, electronic and thermodynamic properties of the ternary cubic filled skutterudite CeOs4Sb12 compound were calculated using the full-potential linear muffin-tin orbital implementation of density functional theory. The exchange-correlation potential was treated with the local density approximation. The calculated ground state quantities such as the lattice parameter, atomic position parameters of Sb atoms, bulk modulus and its pressure derivative are compared to the available experimental data. We have computed the elastic moduli and their pressure dependence, which have not been calculated or measured yet. The Debye temperature is estimated from the average sound velocity. From the elastic parameter behavior, it is inferred that this compound is elastically stable and brittle in nature. The electronic band structure calculations revealed metallic behavior for the herein studied compound at zero pressure, but under pressure effect, the metallic character disappears and the compound becomes a narrow indirect band gap semiconductor. Through the quasi-harmonic Debye model, in which phononic effects are considered, the effect of pressure P and temperature T on the lattice constant, bulk modulus, heat capacity, thermal expansion coefficient and Debye temperature are investigated.

Keywords

Ab-initio; Elastic properties; Electronic properties; Debye temperature; Filled skutterudite