World Academy of Science, Engineering and Technology
International Journal of Materials and Metallurgical Engineering
Vol:8, No:07, 2014

Elastic and Thermal Behaviour of LaX (X= Cd, Hg) Intermetallics: A DFT Study

Authors : Gitanjali Pagare, Hansa Devi, S. P. Sanyal

Abstract : Full-potential linearized augmented plane wave (FLAPW) method has been employed within the generalized gradient approximation (GGA) and local spin density approximation (LSDA) as the exchange correlation potential to investigate elastic properties of LaX (X = Cd and Hg) in their B2-type (CsCl) crystal structure. The calculated ground state properties such as lattice constant (a0), bulk modulus (B) and pressure derivative of bulk modulus (B') agree well with the available experimental results. The second order elastic constants (C11, C12 and C44) have been calculated. The ductility or brittleness of these intermetallic compounds is predicted by using Pugh's rule B/GH and Cauchy's pressure (C12-C44). The calculated results indicate that LaHg is the ductile whereas LaCd is brittle in nature.

Keywords : ductility/brittleness, elastic constants, equation of states, FP-LAPW method, intermetallics
Conference Title : ICMSCMP 2014 : International Conference on Material Science and Condensed Matter Physics
Conference Location : Zurich, Switzerland
Conference Dates : July 30-31, 2014