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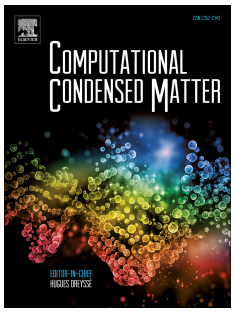

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Study of Structural, Elastic, Electronic, Mechanical, Optical and Thermodynamic Properties of $NdPb_3$ intermetallic compound: DFT Based Calculations

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Abstract

In this paper, we have study the structural, elastic, electronic, mechanical, optical and thermodynamic properties of $NdPb_3$ intermetallic compound using density functional theory (DFT) with CASTEP code for the first time. The structural and other physical properties of $NdPb_3$ compared with the results where available and show well accord. The optimized lattice parameters show a good agreement with the experimental data. The elastic constants C_{ij}, bulk modulus *B*, shear modulus *G*, Young's modulus *Y* and Poisson's ratio *v* are optimized and discussed by using the Voigt-Reuss-Hill (VRH) approximation. The elastic constants show that $NdPb_3$ is a mechanical stable compound. Cauchy pressure, Pugh's ratio and Poisson's ratio indicate that $NdPb_3$ is also a ductile compound associated with ionic bonding nature. Zener's anisotropy index and universal anisotropic index show the anisotropic characteristics of this compound. The density of states (DOS) at Fermi level is high which is mainly contributed by Nd 4*f* indicates the metallic behavior of this compound. The metallic behavior also characterized by band structure and conductivity. This compound is a good reflector at low energies also have a good quality of absorption at visible region. We also determined the Debye temperature from elastic constants, minimum thermal conductivity, melting temperature sound velocities and $Dulong - Petit\ limit$.

Keywords: $NdPb_3$, Structural, Mechanical, Electronic, Bonding analysis, Optical and Thermodynamic Properties.

1. Introduction

Most of the RB_3 (R = rare earth elements or Y, B= In, Sn, Tl, Pb and Ga) types intermetallic compounds crystallize the $AuCu_3$ type cubic crystal structure with space group *pm-3m* (No. 221) where R atoms occupied corner sites and B atoms occupied face centered sites [1-3]. The rare-earth based intermetallic compounds exhibit strong electron correlations due to the incomplete 4*f*shell of the rare-earth elements [4]. The physical properties of these compounds can be determined by the unpaired electron in the incomplete 4*f* shell of rare earth elements [5-6]. These compounds possess several properties including valence fluctuations, gap states, Kondo lattice, quadrupolar ordering, spin and charge orderings, unconventional superconductivity, heavy Fermions (heavy electrons), high melting point, high temperature ductility, high temperature mechanical properties, and good electrical and magnetic properties. The magnetic properties are given by the *f* -Localized model and the absence of *d* electrons at Fermi level shows the ductile nature. Due to these interesting properties these compounds are used in automobile, aviation, aircraft turbines and aerospace application [7-11].