International Journal of Advanced Technology & Engineering Research (IJATER)
International Conference on "Recent Advancement in Science & Technology" (ICRAST 2017)

ELECTRONIC AND MAGNETIC PROPERTIES OF CUBIC REHG (RE = ND AND SM) INTERMETALLIC: A FIRST-PRINCIPLES DFT STUDY

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ABSTRACT

Spin polarized ab-initio calculations have been carried out to study the electronic and magnetic properties of REHg (RE = Nd and Sm) intermetallic compounds in B_2 crystal structure. The calculations have been performed by using both generalized gradient approximation (GGA) and local spin density approximation (LSDA). The calculated values of lattice constant a_0 are found to be 3.686 Å and 3.706 Å respectively for NdHg and SmHg with LSDA, and are in good agreement with the experimental data. The bulk Modulus (B = 63.69 GPa and 60.93 GPa), first order derivative of bulk Modulus (B' = 4.68 and 6.02) and magnetic moment (μ_B = 3.719 and 5.896) are also calculated respectively for both REHg compounds. The band structure and density of states are plotted which reveal the metallic nature for both compounds.

Keywords: Ab- initio Calculation, Electronic properties, Band structure, Magnetic moment.

Introduction

The intermetallic compounds with B_2-type structure have intensely attracted considerable attention, due to their physical and mechanical properties that are often superior to ordinary metals, such as high strength, melting at high temperature, low specific weight, and good corrosion resistance [1, 2]. Intermetallic compounds are amongst the most important solid state materials because of their diverse physical properties and widespread use in numerous applications. These intermetallics can be denoted as the chemical formula RM, where R indicates
a rare-earth element, and M indicates a late transition metal or an early p-element. However, most intermetallic compounds exhibit brittle behavior at room temperature, which limits their engineering applications, in both single crystal and polycrystalline states. In 2003, a new class of high ordered, ductile intermetallic compounds with B_2 structure was discovered by Gschneidner et al. [3]. A well-known property of the rare earth elements is their incomplete 4f shell, which becomes progressively filled in going from La to Lu. The shielding of the 4f shell leads to interesting physical properties which differ from one lanthanide ion to the next by the number of electrons compacted in the 4f shell. Rare earth based intermetallics REHg (RE = Nd and Sm) are binary intermetallic compounds with CsCl structure, which belong to Pm3m space group (no 221). Indelli et al. [4] have predicted that these compounds are stable in B_2 phase and calculated the lattice parameters at ambient conditions by using X-ray diffraction technique. Apart from the experimental lattice parameter of these intermetallics no systematic experimental or theoretical results on the structural and electronic properties are available in literature. In the present paper a comprehensive and systematic study related to the structural and electronic, properties for these compounds has been carried out.

Method of Calculation

REHg (RE= Nd and Sm) compound crystallizes in a simple cubic B_2 structure with two atoms per unit cell. It belongs to the *Pm3m* space group with RE atoms occupying the corners of the cube while the Hg atoms occupying the cube faces. First-principles study of the REHg compound was performed by employing full potential linearized augmented plane wave (FP-LAPW) method [5] based on density functional theory within the generalized gradient approximation (GGA) incorporated in the WIEN2k code [6]. It is a variational method that is at present the most successful approach to compute the electronic structure of matter. The density functional theory is derived from the N- particle Schrodinger equation and useful for system of many electrons. The exchange correlation potential is treated with generalized gradient approximations in the scheme of Perdew, Burke and Ernzhof (PBE-GGA) [7], Wu and Cohen (WC-GGA) [8] and Perdew et al. (PBEsol-GGA) [9] to investigate the structural

and electronic properties of REHg compounds. The basis function has been expanded up to Rmt x K_{max} = 7.0, where R_{MT} is the smallest atomic radius in the unit cell and K_{max} gives the magnitude of the largest k vector in the plane wave expansion. The maximum value for partial waves inside the atomic sphere is l_{max} = 10 while the charge density is Fourier expanded up to G_{max} = 12. The self-consistent calculations are converged when the total energy of the system is stable within 10^{-4} Ry. A dense mesh of 1000 k points and the tetrahedral method have been employed for the Brillouin zone integration. The total energies are fitted to Birch equation of state [10] to obtain the ground state properties. The energy band structure and corresponding density of states are prominent quantities that determine the electronic structure of a system. The spin polarized calculation has been performed using LSDA approximation to understand the electronic behavior of REHg intermetallic compound in terms of electronic band structure (BS) and density of states (DOS). Also, it is the most accurate scheme for band structure calculations. It is based on full-potential (linearized) augmented plane-wave ((L) APW) method, one of the most accurate schemes for band structure calculations. We have used an optimized geometry obtained through a self consistent process to investigate the electronic structure of the crystal lattice of the material.

Result and Discussion

Structural Properties

In order to calculate the ground state properties of mercury based intermetallic REHg (RE = Nd and Sm), the total energies are calculated as a function of reduced volume in B_2-type (CsCl) structure using full potential linearized augmented plane wave (FP-LAPW) method. The equilibrium lattice constant can be obtained by fitting the total energy vs. volume data fitted to the Birch-Murnaghan equation of state. All the results are listed in table 1. REHg compounds are found to be stable in B_2- phase at ambient pressure. An inspection of table 1, reveals that the bulk modulus of NdHg is higher than that of SmHg, indicating that NdHg is harder than SmHg. As shown in table 1, the calculated lattice constants for both the compounds are compared with the available experimental data [5]. The ground state properties, such as equilibrium lattice constant (a_0), bulk modulus (B) and its first derivative (B') for REHg have been calculated in their B_2-phase by the LSDA approximation. We have also found the values of magnetic moment (μ_B) of REHg and presented it in table 1. It is revealed from table 1 that the calculated values of equilibrium lattice constants a_0 are in reasonable agreement with the available experimental data.

Table 1 The calculated structural properties and density of states at the Fermi level $N(E_f)$ for REHg

Solid	Work	Approximation	a_0 (Å)	B (GPa)	B'	$N(E_f)$ *States/eV*	
						Spin Up	Spin Down
NdHg	Present	LSDA	3.686	63.69	4.68	16.20	0.55
		PBE-GGA	3.835	44.77	4.61	-	-
	Experimental	XRD	3.780[a]	-	-	-	-
SmHg	Present	LSDA	3.706	60.93	6.02	14.96	0.49
		PBE-GGA	3.855	40.64	5.35	-	-
	Experimental	XRD	3.744[a]	-	-	-	-

[a]Ref[4]

Electronic Properties

The electronic energy band structures along the principal symmetry directions for REHg in B_2 phase are presented in Fig1 (a) and (b). The band structures are calculated along the path that contains the highest symmetry points in the Brillouin zone, namely R→Λ→Γ→Δ→X→Z→M→Σ→Γ. The energy zero is set at the Fermi level. The lowest lying band in both REHg compounds resulting mainly from '5*d* ' state of Hg. The difference in the spin up and spin down bands is primarily due to the '4*f* ' states. The occupied spin up '4*f* ' states are at the E_f and around 0 eV to 0.6 eV while the spin down 4f states stages gets shifted over the E_f around 2.2 eV and 3.6 eV for NdHg and SmHg respectively.

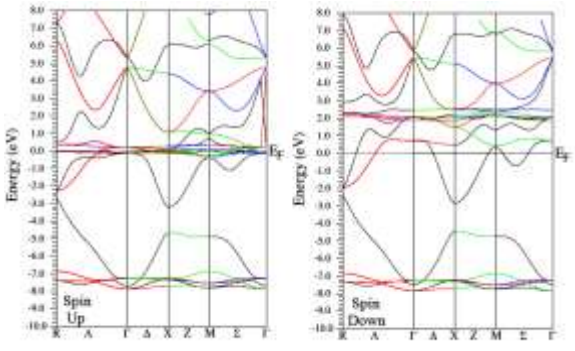

Figure 1(a) Band Structure of NdHg

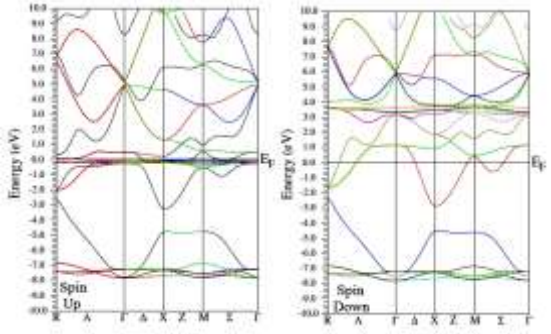

Figure1(b) Band structure of SmHg

To further reveal the nature of the electronic band structures and the bonding situation, we have also calculated the total and partial density of states (DOS) for REHg and presented in Fig 2(a) and (b). At the Fermi level, the bands are crossing the Fermi level from valence band to conduction band ,hence exhibiting the metallic behavior. The '4*f* ' states are easily identified as sharp peaks in the total DOS. Generally, the '4*f* ' states are highly localized and lie at or close to E_f in REHg compounds. The valence band mainly consists of '*d* ' state of Hg atoms. The delocalized '4*f* ' states of RE are situated between 0 eV to 0.4 eV around Fermi level for NdHg in spin up channel, but it gets shifted between 2 eV to 3 eV above the Fermi level in conduction band in spin down channel. For SmHg the 4f states originate from -0.2 eV to 0.4 eV in spin up mode whereas for spin down channel it gets shifted to 3.4 to 4.0 eV in conduction band. The metallicity in both the REHg compounds is due to '4*f* ' states of RE with little contribution of '5*d*' state of Hg atoms. The finite values of DOS at the Fermi level for both REHg compounds are listed in table 1.

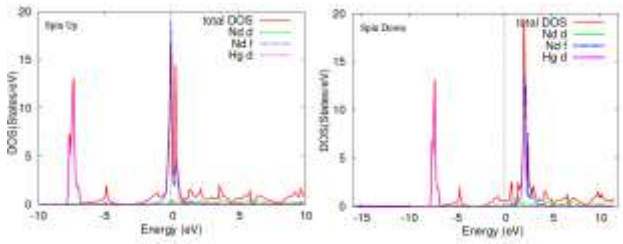

Figure 2(a) The Density of States of NdHg

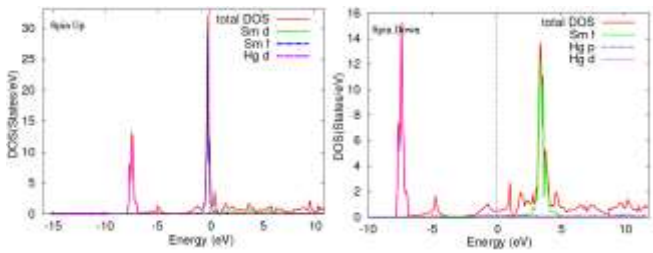

Figure 2(b) The Density of States of SmHg

Conclusion

In this work, We have investigated the structural and electronic properties of REHg (RE = Nd and Sm) compounds. We have systematically studied these compounds by using the FP-LAPW method based on density functional theory, within different Schemes of approximations, LSDA and PBE-GGA as the exchange correlation potential. The electronic properties of these compounds are studied by calculating band structures and its corresponding density of states. The electronic band structure calculation shows that all the studied compounds have zero band gap values and show metallic nature.

Acknowledgement

The authors are thankful to MPCST (M. P. Council of Science and Technology) for the financial support.

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