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First – Principles Study on Ground State Properties and Electronic Structure of Binary Rare Earth Intermetallic Compounds: NdCd and SmCd

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Abstract *– First principles study on ground state properties and electronic structure of binary cadmium based rare earth intermetallics have been carried out using the full–potential linearized augmented plane wave method (FP-LAPW) within density functional theory (DFT). Results on structural properties are obtained using generalized gradient approximation (GGA) and local density approximation (LSDA). The equilibrium lattice parameter (a_0), bulk modulus (B), its pressure derivative (B') and magnetic moment (μ_B) have been obtained using optimization method. Our calculated results agree well with available experimental results. From band structure and density of state calculations, it is found that both NdCd and SmCd exhibits metallic behavior. Density of states (DOS) at the Fermi level (E_F) for NdCd and SmCd for majority spin is found to be 8.44 and 10.25 states/eV, while for minority spin 0.50 and 0.581 states/eV values are calculated respectively for NdCd and SmCd. This is the first prediction of electronic spectra of NdCd and SmCd intermetallics.*

Keywords*: Density Functional Theory, Ground state properties, Electronic properties*

I. Introduction

Intermetallic compound consist of two or more metals combined with specific stoichiometries by mixed metallic, covalent and ionic bonding. Rare earth intermetallics have many attractive properties such as, high oxidation and corrosion resistance, thermal stability and relatively low densities, combined with their ability to retain strength and stiffness at elevated temperatures, which makes them promising high temperature structural material for automobile, aviation and aerospace application [1-5].The intermetallic compounds have emerged as materials with vast potential for application in a wide range of technologically important areas. Rare earth intermetallics have unusual physical and electronic properties. Rare earth compounds have partially filled *f* electron orbital. The *f* electrons in the rare earth ion are highly delocalized and under the effect of pressure they interact strongly with the conduction band and with the *p* -states of the neighboring anion. Due to this the rare earth compounds shows interesting electronic, optical and magnetic properties. Light rare earths like Ce, Pr, Nd and Sm have weakly delocalized *f* states where as heavier rare earth have strongly localized *f* states. Pinto *et. al*. [6] have studied the electrical and thermoelectric transport properties of RZn and RCd compounds (R= Tb, Gd, Nd and Pr) between 4.2 to 300 K and found that these compounds exhibit ferromagnetism below room temperature. Magnetic properties of CeCd and NdCd single crystals have been reported by Fujii *et. al.* [7], they found that there are two successive structural transitions about T_{S1}=100K and T_{S2}=210K in CeCd and a ferromagnetic to paramagnetic phase transition appears at Tc=16.5K, while NdCd does not show any structural instability above Tc=121 K. Both NdCd and SmCd have B_2 type (CsCl) structure in which Cd atoms are positioned at the center of the cubic cell (0.5, 0.5, 0.5) and Nd and Sm atoms occupy (0, 0, 0) positions at the corners of the cubic cell belonging to space group (*Pm*3*m*) of number 221 [8] respectively. Phase diagram of samarium- cadmium system has been studied by Bruzzone *et. al.* [9]. The mixing of rare earth with Cd has made a new class of highly ordered and ductile compounds. It is evident from the literature that the role of *f* -electron in rare earth ion with Cd in structural and electronic properties at normal and high pressure has not

been extensively studied and is yet to be explored in detail. A theoretical study of structural, electronic, elastic and thermal properties of YX (X= Cd, In, Au, Hg and Tl) intermetallics has been performed by Chouhan *et. al.* [10] using first principles density functional theory based on full potential linearized augmented plane wave (FP-LAPW) method. In the rare earth intermetallics *f* – electrons play a crucial role in exploring structural and electronic properties. Therefore, it becomes important to understand the electronic properties of this class of intermetallics. In the present work, spin polarized calculations are performed to investigate the fundamental properties of the TbCd with B_2 structure using generalized gradient approximation (GGA) of PERDEW, BURKE and ERNZRHOF (PBE) [11] and Local spin density approximation LSDA approximations[12]. We report the ground state properties and electronic structure of NdCd and SmCd at ambient pressure. The rest of the paper is organized as follows: section 2 deals with the method of calculations which is employed for the ground state properties of the NdCd and SmCd intermetallic compound. In Section 3, we present the electronic spectra including band structure and density of states. Finally, we present the conclusion in Section 4.

II. Method of Calculation

The calculation have been performed in the frame work of Density functional Theory (DFT).We have employed the full- potential linearized augmented plane wave method as implemented in the WIEN 2K code [13]. In the FP-LAPW method, the wave function, charge density and potential are expanded by spherical harmonic functions inside non-overlapping spheres surrounding the atomic sites (muffin-tin spheres) and by a plane wave basis set in the remaining space of the unit cell (interstitial region). In order to achieve the energy eigen value convergence, we expand the basis function up to $R_{MT}*K_{max}= 7$ where R_{MT} is the smallest atomic sphere radius in the unit cell and K_{max} gives the magnitude of the largest *K* vector in the plane wave expansion. The valence wave functions inside the spheres are expanded up to l_{max} =10 while the charge density is Fourier expanded up to G_{max}= 12. The self-consistent calculations are considered to converge when the total energy of the system is stable within 10^{-4} Ry. A dense mesh of 1000 **k** points is used and the tetrahedral method has been employed for the Brillouin zone integration. The total energies are calculated as a function of volume and fitted to Birch equation of state [14] to obtain the ground state properties.

III. Results and Discussion

III.1. Structural Properties

The spin polarized electronic band structure calculations have been carried out to obtain the total energy of the NdCd and SmCd intermetallic compounds using the first principles FP-LAPW method. In order to calculate the ground state properties, the total energies are calculated in B_2 phase for different volumes around the equilibrium cell volume V_0. The variation of total energy as a function of volume for these compounds is shown in Fig1 (a) - (d). The calculated total energies are fitted to the Birch–Murnaghan equation of state [14] to determine the ground state properties like lattice constant (a_0), bulk modulus (B) and its pressure derivative (B') and magnetic moment (μ_B) at minimum equilibrium volume V_0 using exchange correlation as GGA [11] and LSDA [12] . The calculated ground state properties like lattice constant (a_0), bulk modulus (B), its pressure derivative (B') and magnetic moments (μ_B) are given in Table 1, and compared with the experimental data [8]. It is seen from Table 1 that our calculated values of lattice constants (a_0) are in good agreement with the available experimental result [8]. The lattice parameters calculated by both GGA and LSDA agrees well with experimental result. This demonstrates that the computational methodology employed in this work is suitable. From Table 1, one can see that the GGA leads to larger lattice parameter than the LSDA. This is because the LSDA leads to strong overbidding which results too small lattice parameter while GGA corrects the over binding tendency inherent in LSDA [15].

TABLE I
Calculated ground state properties such as lattice parameter, bulk modulus its pressure derivative and magnetic moment for NdCd and SmCd.

Solid	Work	a_0 (A°)	B (GPa)	B'	μ_B
NdCd	LSDA	3.718	52.75	4.58	3.91
	GGA	3.867	44.85	4.10	3.86
	Expt.	3.811[a]	-	-	-
	Theo.	-	-	-	-
SmCd	LSDA	3.730	52.61	4.43	5.93
	GGA	3.888	36.18	4.24	5.89
	Expt.	3.771[a]	-	-	-
	Theo.	-	-	-	-

[a] Ref [8]

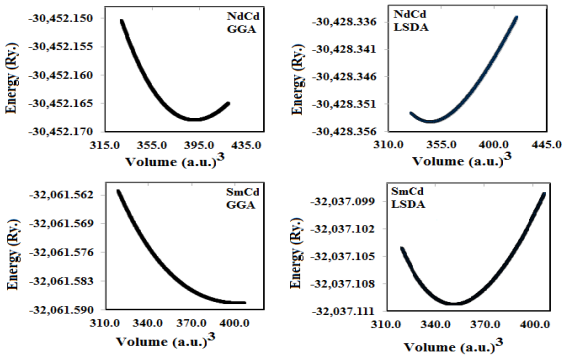

Fig. 1.Variation of total energy vs. relative volume of NdCd and SmCd using GGA and LSDA approximations.

III.2. Electronic Properties

The self consistent spin polarized electronic band structure along the high symmetry direction for majority and minority spins for NdCd and SmCd intermetallics are presented in figure 2 (a)- (d). The total and partial density of states (DOS) at ambient pressure and presented in figure 3 (a) - (h) by using LSDA approximation. The Fermi Level (E_F) is considered at origin. Since conduction band and valence band are overlapping at the Fermi Level (E_F), suggesting the metallic nature of these intermetallics. It is seen from figure 2 that the bands lie about -8.0 eV in these intermetallics are due to the '*d*' like states of Cd in both the spin channels. The cluster of bands, which are situated at the Fermi level, are mainly due to the itinerant '*f*'-bands of RE (Nd, Sm) for majority spin channel of these compounds resulting in metallic behavior.

The density of states (DOS) plot provides an even more comprehensive picture of the elemental contributions to the electronic structure of these compounds. In case of NdCd, for majority spin channel, the '*f*' like states of Nd lies at the Fermi level (E_F) and is hybridized with the'*d*' states of Nd and '*p*' states of Cd. Hence the major contribution of DOS at the Fermi level is due to the '*f*' like states of Nd. For minority spin channel these states get shifted and lie in the conduction region. Density of states for majority and minority spin channel is found to be 8.44 and 0.5 states/eV respectively. For SmCd, '*f*' like states of Sm are situated at the Fermi Level with a little admix of'*d*' states of Sm and '*p*' states of Cd. Finite DOS at the Fermi Level in spin up channel show the metallic character of this compound with a DOS value of 10.25states/eV while for spin down channel it is found to be 0.58 states/eV. Since density of states measure the electronic density which is the main cause of electrical conductivity and main cause of electrical conductivity on these intermetallic is the 'f' states of rare earth atoms.

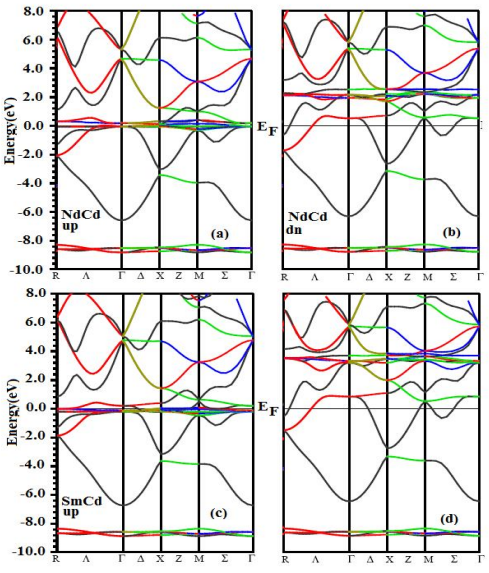

Fig. 2. Band structures of NdCd and SmCd using LSDA approximation.

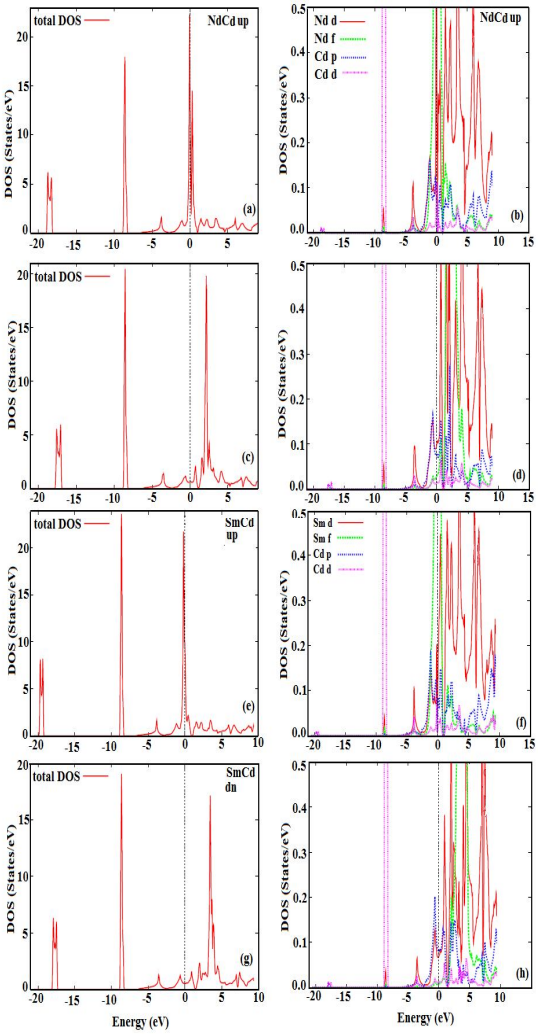

Fig. 3 Density of states (DOS) for NdCd and SmCd using LSDA approximation.

IV. Conclusion

In conclusion, we have systematically studied the structural and electronic properties of the B_2- type (CsCl) NdCd and SmCd rare earth intermetallic compounds using FP-LAPW method based on density functional theory. The ground state properties such as lattice parameter (a_o), bulk modulus (B) its pressure derivative (B') and magnetic moment (μ_B) are computed and compared with the available experimental result which shows good agreement. We have also computed the electronic spectra for these compounds which show that these intermetallics are metallic in nature. The importance of present study is that it may provide a new insight to future experimentalists and theoreticians on such a dynamic materials to look at their electronic properties.

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References

[1] Y. Wu, W. Hu, European Physical Journal B, 60, 2007.

[2] M. Divis, J. Kriplach, *Physica B,* 205, 353-364, 1995.

[3] L. Chen, P. Peng, S. C. Han, *Rare Metal Materials and Engineering,* 36, 2089, 2007.

[4] S. K. Pasha, M. Sundareswari and M. Rajagopalan, *Physica B,* 348, 206-212, 2004.

[5] A. Ricca, C. W. Bauschlicher, *Chemical Physics,* 200, 337.

[6] H. Fujii, T. Kitai, Y. Uwatoko and T. Okamoto *Journal of magnetism and magnetic material,* 52, 428-430, 1985.

[7] A. Indelli and A. Palenzona, *Journal of the less common metal,* 9, 1-6, 1965.

[8] G. Bruzzone and M.L. Fornasini, *Journal of the less Common metal,* 37, 289-292, 1974.

[9] Sunil Singh Chouhan, Gitanjali pagare, M. Rajagopalan and S. P. Sanyal, *Solid State Sciences* 14, 1004 – 1011, 2012.

[10] J. P. Perdew, K. Burke, M. Ernzerhof, *Physical Review Letter,* **77,** 3865-3868, 1996.

[11] P. Hohenberg, W. Kohn, *Physical Review,* 136, *B*864-B871, 1964.

[12] F. Birch, *Phy. Rev.*71, 809-824, 1947.

[13] J. Hafner, *Journal of Computational Chemistry* 29, 2044-2078, 2008.

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