

STRUCTURAL AND ELECTRONIC PROPERTIES OF REOS₂ (RE=SM, GD) MGZN₂-TYPE LAVES PHASE COMPOUNDS

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Abstract- The structural and electronic properties of rare earth REOs₂ (RE=Gd and Sm) Laves phase compounds were studied using density functional theory. For exchange and correlation effect, we have used LSDA and LSDA+U approximations. These compounds are crystallizes in MgZn₂-type hexagonal structure. Ground states properties are calculated and compared with the available experimental data. Band structures and density of states reveal that these compounds are metallic in nature.

Keywords – Laves Phase Compounds, Electronic Structure, Density Functional Theory, Hubbard Parameter

1. INTRODUCTION

Rare earth Laves phase compounds are growing interest due to their excellent physical and chemical properties that make them available for several functional and structural applications. These types of intermetallic compounds are classified as a Laves phase on the basis of their geometry of the crystal structure. Although AB₂ type Laves phase compounds crystallize in three different structures namely face centered C15 (MgCu₂), hexagonal C14 (MgZn₂) and di-hexagonal C36 (MgNi₂). The rare earth REOs₂ (RE= Sm, Gd) are crystallize in either C15 (MgCu₂-type) or C14 (Hexagonal MgZn₂-type) structure. It has been observed that light rare earth RE's (La-Pr) are formed with C15 phase and heavier rare earth RE's (Pr-Lu) are formed with C14 phase [1]. An orthorhombic structure also exists, where observed a number of intermetallics, namely CeCu₂-type structure also exist. Since Friauf, was the first one to study the crystallographic structures of MgCu₂ and MgZn₂, these intermetallic phases are also referred to as 'Friauf-Laves phases' [2]. Canon et. al [3] have reported the effect of high pressure on the crystal structure of LaOs₂ and CeOs₂ Laves phase compounds using experimental techniques. Torikachvili et. al [1] have investigated the low temperature properties of CeOs₂ in the C14 and C15 crystallographic Laves phases compounds using X-Ray diffraction. Magnetizations of Compounds of Rare Earths with Platinum Metals have reported by Bozorth et. al [4]. The structural and magnetic properties on Laves Phase Compounds of Rare Earths and of Hafnium with Noble Metals have been studied by Vera et. al [5].using X-Ray diffraction.

The present paper is concentrated on hexagonal C14 (MgZn₂) type Laves phase REOs₂ (RE=Sm, Gd) compounds. The structural and electronic properties of Osmium based compounds in hexagonal C14 (MgZn₂-type) phase are calculated and presented for the first time.

The rest of the paper is organized as follows. The second section describes the computational details. Results on structural and electronic properties are reported and discussed in the third section.

2. METHOD OF CALCULATION

For calculating the structural and electronic properties of REOs₂ (RE = Gd, Sm) intermetallic compounds, we have used full potential linearized augmented plane wave (FP-LAPW) method as implemented in the WIEN2k code [6] within local spin density approximation (LSDA) and LSDA+U (U-Hubbard and exchange parameter) [7,8]. These compounds crystallize in MgZn₂-type structure with space group P63/mmc (No. 194) where the rare earth (Gd and Sm) are located at (0.3333, 0.6667, 0.063) and Os1 and Os2 atoms are located at (0, 0, 0), (0.833, 0.666, 0.250). The energy eigen value convergence was achieved by expanding the basis function up to RMT*Kmax= 7, where RMT is the smallest atomic sphere radius in the unit cell and Kmax gives the magnitude of the largest k vector in the plane wave expansion. The valence wave functions inside the spheres are expanded up to lmax = 10 while the charge density is Fourier expanded up to Gmax = 12. The self consistent calculations are considered to converge when the total energy of the system is stable within 10⁻⁴ Ry. Energy to separate core and valence state is -6.0 Ry. Integration in the Brillouin zone was performed using k-points generated with 7×7×3 mesh points. To calculate the accurate results and due to the presence of localized (4f- electrons) in RE (RE=Gd and Sm) atoms, we have used LSDA+U (U-Hubbard and exchange parameter). In the LSDA +U calculations, we have used an effective parameter U_{eff} = U-J, where U is Coulomb interaction (Hubbard) parameter and J is exchange parameter. The values of Hubbard (U= 6.70 eV (Gd), U=6.90 eV (Sm) and 3.4 eV (Os) and exchange parameter (J = 0.70 eV) are taken for these atoms.

3. RESULTS AND DISCUSSION

3.1 Structural properties–

The spin-polarized calculation has been performed to obtain the ground state properties of REOs₂ (RE=Sm and Gd) Laves phase compounds using LSDA and LSDA+U approximation. For the determination of static equilibrium properties of REOs₂ (RE=Sm and Gd) Laves phase compounds, we have used the Birch-Murnaghan's equation of state [9]. The obtained equilibrium lattice constants (a_0), Bulk modulus (B_0), its pressure derivatives (B_0') and total magnetic moments are presented in Table 1 together with the available experimental results. It is seen from Table 1

Table 1. Structural and electronic properties of SmOs₂ and GdOs₂ Laves phase compounds

Solids	Appr.	Lattice parameter a_0 (Å)	c_0 (Å)	Bulk Modulus B_0 (GPa)	B_0'	N(EF) (States/eV)		Total Magnetic Moment
						↑	↓	
SmOs ₂	LSDA	5.252	8.749	230.4	4.64	-	-	27.42
	LSDA+	5.253	8.752	229.4	4.73	33.3	5.77	26.82
	Expt.	5.336 ^{a,b}	8.879 ^{a,b}					
GdOs ₂	LSDA	5.248	8.714	240.6	3.60	-	-	20.95
	LSDA+	5.241	8.700	243.1	4.44	5.17	9.26	21.42
	Expt.	5.319 ^{a,b}	8.838 ^{a,b}					

a Ref [5] ; b Ref [10]

that our calculated results are in good agreement with the experimental data.

3.2 Electronic Properties –

The calculated electronic band structure along the principle symmetry directions of SmOs₂ and GdOs₂ rare earth Laves phase compounds using LSDA+U approximations are presented in Figs.1 (a)-(b) for spin up and spin down respectively. The lowest lying bands in SmOs₂ and GdOs₂ around -10.0 eV - -8.0 eV are mainly due to '6s' states of Os and the bands below the EF are mainly composed due to 'd' states of Os and 'd' states of RE (RE=Sm, Gd) atoms.

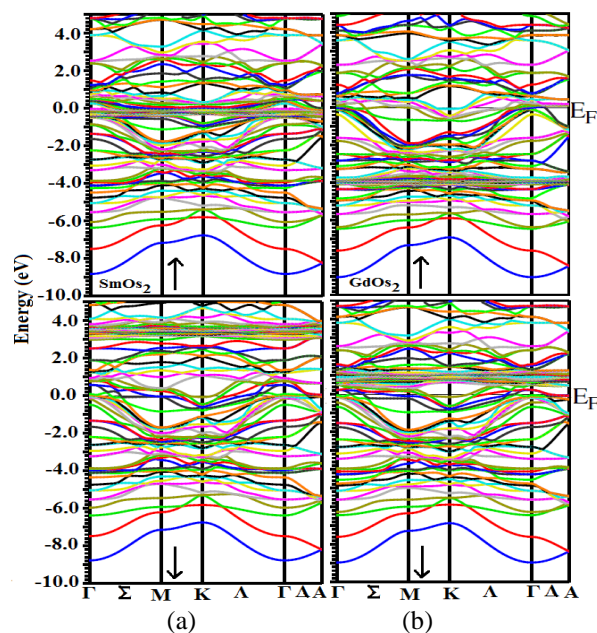


Figure 1. Electronic band structure for (a) SmOs₂, (b) GdOs₂

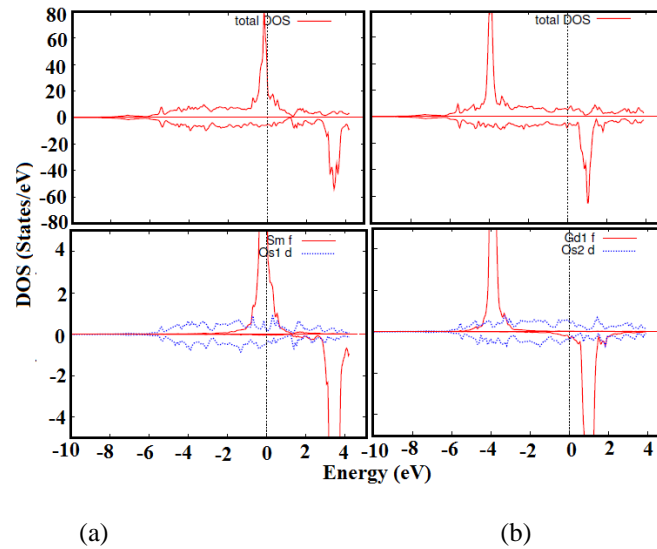


Figure2. Total and Partial density of states for (a) SmOs₂, (b) GdOs₂

The band profile of majority and minority spins are quite similar except the localized RE-f states at the Fermi level are shifted to the conduction bands around the energy range 3 to 4 eV in case of SmOs₂ while in GdOs₂, the flat bands are localized below the Fermi level around -4.0 eV in spin up channel is shifted to the conduction band side in spin down channel.

The localized flat bands or cluster can also be seen in DOS profile (Fig. 2(a)-(b)) for SmOs₂ and GdOs₂ compounds. Here the sharp peaks are mainly due to 'f' states of RE atoms. RE-'f' states and Os-'d' states are mainly contribute in band structures. The density of states at the Fermi level shows the metallic nature present in these compounds in both spin channel. The density of states at Fermi level $N(E_F)$ and magnetic moments are presented in Table.1 for both spin channels.

4. CONCLUSION

We have performed the first principle studies to calculate the structural and electronic properties of rare earth Laves phase compounds. The lattice parameters are in agree well with previously reported results. The localized RE-'f' state can be seen below or at the Fermi level (valance region) in spin up channel and above the Fermi level (conduction region) in spin down channel. The band structures show the metallic nature present in these compounds.

5. REFERENCE

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