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Research Article

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First principles study of full Heusler Rh_2TiGe compound

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ABSTRACT

Spin Polarized Band Structure calculation of Rh_2TiGe compound is reported for the first time using FP-LAPW method treated with PBE-GGA exchange correlation. The percentage error in optimized lattice parameter is found to be 1.2%. This material is found to be metallic and diamagnetic. Near Fermi Energy level is mainly occupied by Rh-d and Ti-d-electrons. Bulk modulus and magnetic moment values are reported.

Keywords: Heusler compounds, Diamagnetic, Band structure, Density of States, metallic bonding.

INTRODUCTION

The discovery of Heusler alloys (1) has revolutionized the research field as one could derive potential candidates for multifunctional applications. Full Heusler alloys with L21 structure and Cb1 structure have been studied (2, 3, 4) mainly for its half metallic character and some of them are found to be ferromagnetic with 100 % spin polarized. Many such Heusler alloys are explored and reported to be spintronic (5, 6) materials. The half Heusler alloys (7, 8) have also been prepared and reported by many researchers. MgAgAs structured half Heusler alloys are found to be thermo electric materials. GilleBen (10) has theoretically predicted and reported many full and half Heusler compounds using Density Functional Theory. In the interest to study the structural property of one such predicted compound, Rh_2TiGe compound has been chosen. To the best of our knowledge, we report here for the first time, its band structure, DoS histograms and charge density plot in order to explore their electronic transport behavior and chemical bonding between their atoms.

COMPUTATIONAL DETAILS

An augmented plane wave plus Local Orbitals program as implemented in the wien2k (11) code using Density Functional Theory (12) has been applied in order to study the band structure calculations of the compound Rh_2TiGe. PBE-GGA (Perdew-BurKe-Ernzerhof96) (13) exchange correlation potential is used. The Muffin Tin radius of Rh, Ti and Ge are 2.44a.u, 2.35a.u and 2.40a.u respectively. The number of k-points chosen are 1000 but only 47 irreducible points have been generated. The cutoff parameter are $Rk_{max}=7$, $l_{max}=10$, $G_{max}=12$ a.u^{-1}. The space group of full Heusler alloy is 225 with four inter penetrating FCC lattices. The chemical formula of the full Heusler alloy is X_2YZ where X and Y atoms are transition metals and Z atoms are main group (Al,Si,Ga,Ge,...) elements. The X atoms occupy (¼, ¼ , ¼) and (¾,¾ , ¾), Y atoms at (½, ½,½) and Z atoms at (0,0,0). XCrySDen (14) package has been used to plot the crystal structure of Rh_2TiGe and is shown in Figure1.

RESULTS AND DISCUSSION

A structure file has been generated for the compound Rh_2TiGe with the reported lattice parameter (10). The volume optimization has been carried out in order to get the minimum total energy using SCF with energy convergence of 0.0001 Ry and charge convergence of 0.0001e. The calculated total energy was fitted into the Murnaghan's equation of state (15). The volume optimized curve is presented in Figure2. The details of optimized lattice parameter and bulk modulus are given in Table1. The optimized lattice parameter matches well with the already reported (10).

Table1:

Lattice Constant a_0 (a.u)			**Bulk Modulus** B (GPa)	**Equilibrium Total Energy (Ry)**
Theory(10)	Present	% error		
11.6331	11.6317	1.2	198.9644	-25047.049305

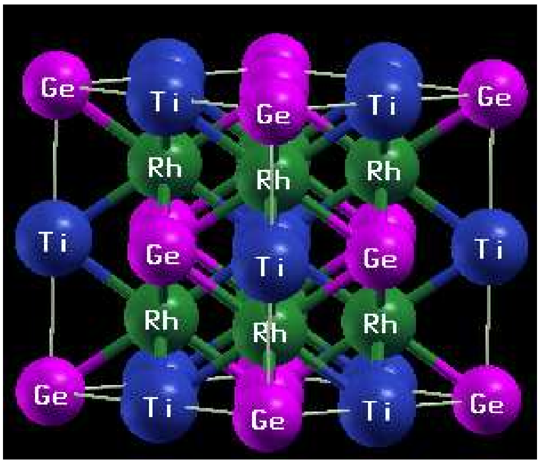

FIGURE1.Crystal Structure of Rh_2TiGe

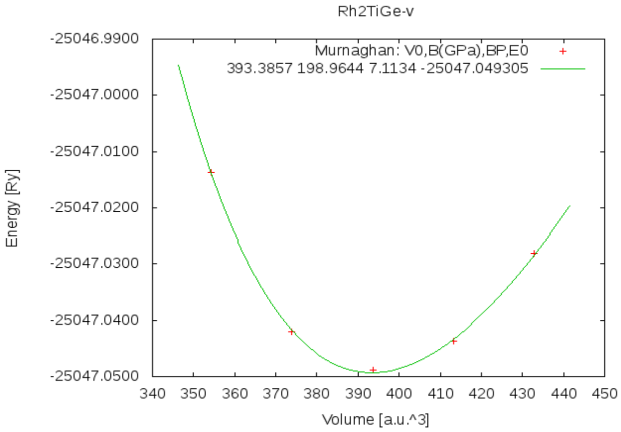

FIGURE2. Total Energy Vs Volume of Rh_2GeTi

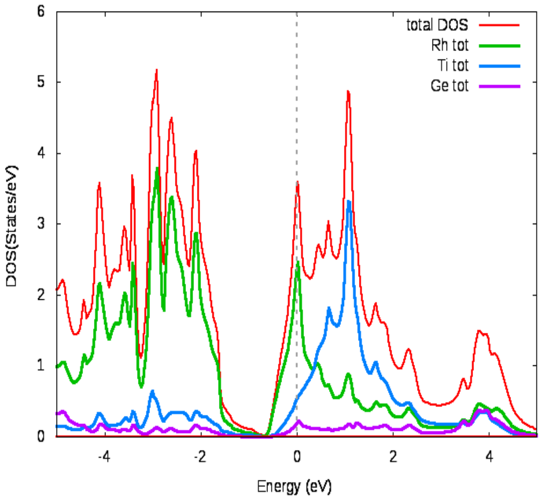

FIGURE.3a.Total DOS of Rh_2TiGe

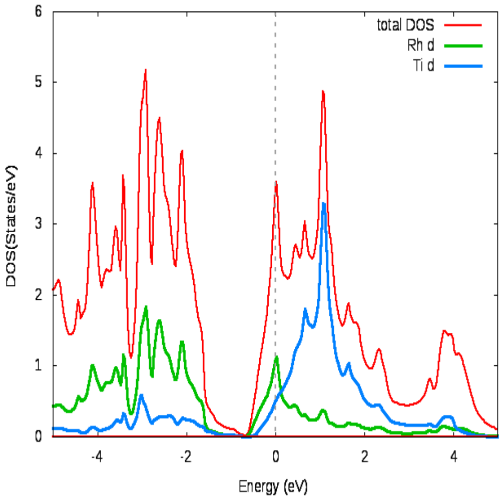

FIGURE.3b.Projected DOS of Rh_2TiGe

The spin magnetic moment of the compound in unit cell is given in Table 2 and since the total spin magnetic moment is negative, one could say that Rh_2TiGe is diamagnetic. The total and projected density of states histograms are drawn and are shown in Figure 3a and 3b. From this plot one can understand that the Density of States (DOS) at Fermi level is predominantly due to Rh-d and Ti-d states; Germanium does not contribute to the DOS at the Fermi Level. Also the d states of Rh and Ti has exchange interaction around the Fermi level. The density of states at Fermi level for spin-up and spin-down is found to be 48.69 and 28.69 respectively. From the band structure that is shown (Figure 4) for Rh_2TiGe, one could state that the compound is metallic in nature as electronic bands from valence band cross the Fermi level and get into the conduction band. From Fig.4(b) and 4(c), it is clear the Rh-d and Ti-d bands shown as fat bands are dominating at the Fermi level. As there are only spherical contours in the electron density plot of Rh_2TiGe (Fig.5) around each atom, the type of bonding between atoms is metallic bonding.

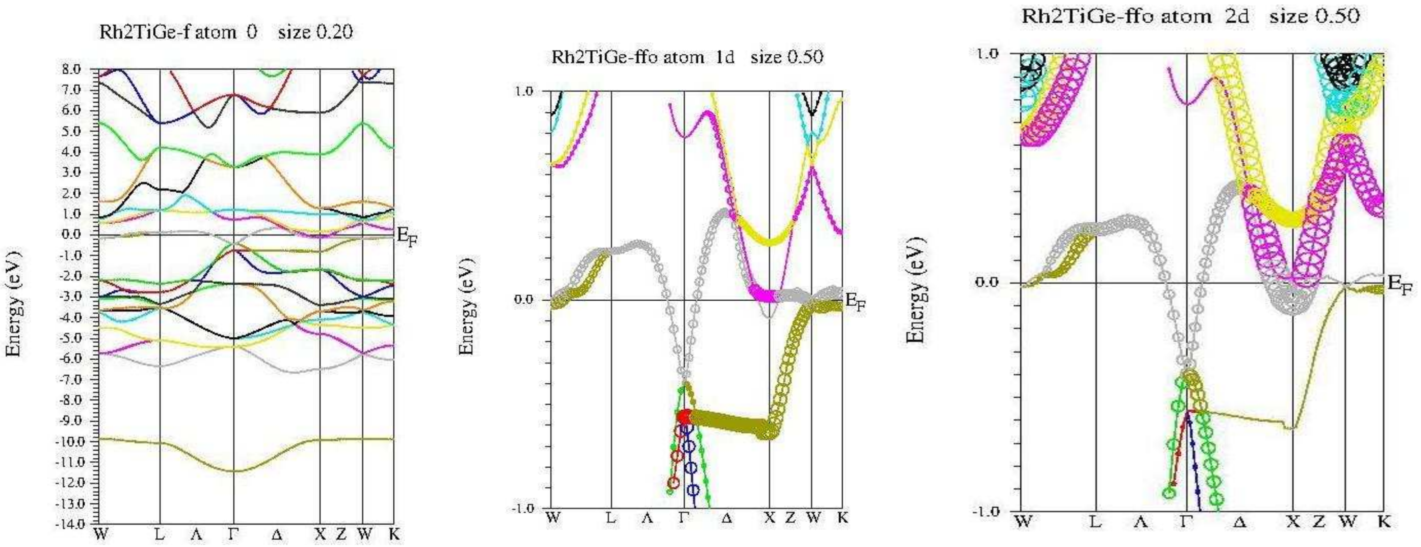

Fig.4(a) **Fig.4(b)** **Fig.4(c)**

FIGURE.4(a-c). Band Structure of Rh_2TiGe.

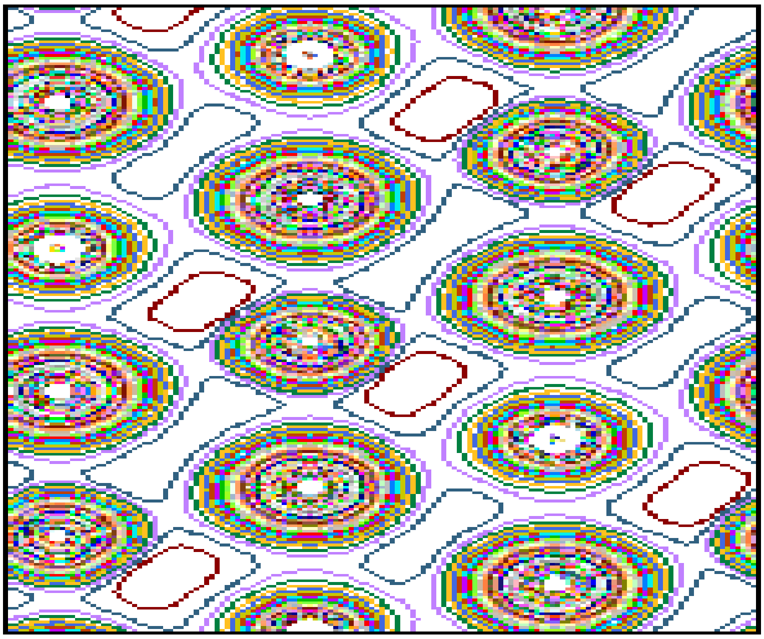

FIGURE 5. Electron Density Plot of Rh_2TiGe

Table 2:

Magnetic Moment of Rh_2TiGe				
Total (reported(10)	**Rh**	**Ti**	**Ge**	**Total (present)**
000	-0.15878	-0.03895	-0.02328	-0.40229

CONCLUSION

The band structure, DoS histograms are drawn for the theoretically predicted compound Rh_2TiGe Heusler compound. Analysis reveals that they are metallic and diamagnetic in nature. Bulk modulus is found to be 199 GPa. It is proposed to do the BoltzTraP calculation to find its resistivity and thermal properties.

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