Band structure and transport studies of half Heusler compound DyPdBi: An efficient thermoelectric material

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Abstract

The discovery of Heusler alloys has revolutionized the research field of intermetallics due to the ease with which one can derive potential candidates for multifunctional applications. During recent years, many half Heusler alloys have been investigated for their thermoelectric properties. The f electron based rare earth ternary half Heusler compound DyPdBi has its f energy levels located close to the Fermi energy level. Other research efforts have emphasized that such materials have good thermoelectric capabilities. We have explored using first principles the electronic band structure of DyPdBi by use of different exchange correlation potentials in the density functional theoretical framework. Transport coefficients that arise in the study of thermoelectric properties of DyPdBi have been calculated and illustrate its potential as an efficient thermoelectric material. Both the theoretically estimated Seebeck coefficient and the power factor agree well with the available experimental results. Our calculations illustrate that it is essential to include spin-orbit coupling in these models of f electron half Heusler materials.

Keywords: Heusler alloys, intermetallic compounds, thermoelectric materials, electronic band structure, spin-orbit effects

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1. Introduction

Intermetallic compounds play a vital role in designing new materials for various technology applications including refractory and structural applications, spintronics and magnetic and superconductivity applications. Ab-initio study on rhodium based intermetallic compounds $\text{Rh}_3\text{X}$ ($\text{X} = \text{Ti}, \text{Zr}, \text{Hf}, \text{V}, \text{Nb}$ or $\text{Ta}$) has been carried out by Rajagopalan, et al [1] at ambient conditions and under compression. The discovery of Heusler alloys [2] has revolutionized the research field on intermetallics, since one can derive potential candidates for multifunctional applications. Full Heusler alloys ($\text{R}_2\text{TX}$ type where $\text{R}$= rare-earth, $\text{T}$= transition metal and $\text{X}$= p-electron element of the periodic table) with $\text{L}_2\text{I}_1$ structure, and half Heusler alloys ($\text{RTX}$ type) with $\text{C}_1\text{b}$ structure, have been studied [3, 4, 5] mainly for their half metallic character. Many such materials are reported to be ferromagnetic; some are spintronic with 100% spin polarization.

Several half Heusler alloys [6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20] have been prepared and reported by experimentalists and also by theoreticians. Gillessen [21, 22, 23] has theoretically predicted and reported many full, and half, Heusler compounds using Density Functional Theory. Band structure calculations on one such Heusler alloy, namely $\text{Ir}_2\text{CrAl}$, have been reported by Krishnaveni, et al [24] which reveal 100% spin polarization, half-metallicity, and ferromagnetism, with a magnetic moment of $3\mu_B$. The properties observed in half Heusler compounds include half metallicity, semiconductivity, giant magnetoresistance, or heavy Fermion state.

Increasing demand for energy necessitates finding alternative ways of generating electricity. Thermoelectric materials generate electric current using the Seebeck effect. The major challenge is the generation of very high thermoelectric current. Over the years many half Heusler alloys have been investigated for their thermoelectric properties. The figure of merit (ZT) value characterizes the efficiency of the thermoelectric property of the given material. $\text{ZT} = \sigma S^2 T/\kappa$ where $T$ is the temperature, $\sigma$ is the electrical conductivity, $S$ is the Seebeck coefficient and $\kappa$ is the thermal conductivity which contains both the electronic and the lattice contributions. Increased efficiency of thermoelectric performance of a given material can be sought by enhancing its Seebeck coefficient, its electrical conductivity or lowering its electronic/lattice thermal conductivity. That can be attained by tuning the
Mahan and Sofo \cite{26} have reported that if the f-levels of any given system lie close to the Fermi level, then that system has good thermoelectric response. That motivates us to consider an f-electron based rare earth (R) ternary half Heusler compound, namely DyPdBi, which has been synthesized and reported earlier \cite{15}. This compound DyPdBi crystallizes \cite{15} in the cubic structure of MgAgAs type, with the space group 216 (F-43m) where Dy occupies the position (0, 0, 0), Pd occupies position (3/4, 3/4, 3/4), and Bi occupies the (1/2, 1/2, 1/2) position \cite{12}. Experimental investigations \cite{15} show that DyPdBi is antiferromagnetic up to 3.5K, exhibits metallic behaviour at low temperature and is semiconducting at high temperature.

In this paper, we report the electronic and transport properties of the DyPdBi compound as predicted by first principles electronic band structure calculations. Although much theoretical work has been reported for quite a number of thermoelectric materials, f-electron systems have not been explored extensively to the best of our knowledge. As one has to compare and look for possible accord between the existing experimental results for DyPdBi with that of the theory of strongly correlated f-electron systems, to begin with we performed band structure calculations on DyPdBi by applying different exchange correlation potentials. In order to study the thermoelectric properties of DyPdBi, the transport coefficients have been calculated by using Boltzmann theory. The BoltzTraP code, developed by Madsen and Singh \cite{27} as implemented in the Wien2k package, was used to calculate the Seebeck coefficient, power factor, and other transport coefficients.

2. Computational Details

First principles band structure calculations have been performed on the DyPdBi compound using the full potential linear augmented plane wave (FP-LAPW) method with PBEsol-GGA (Perdew etal-08) exchange correlation as implemented in the Wien2k (13.1) code \cite{28} by generating the structure file with an experimental lattice parameter \cite{15} of $a_{\text{exp}} = 12.5388$ a.u. The FP-LAPW method includes a procedure for solving Kohn-Sham equations for the ground state density, total energy and eigenvalues of a many electron system by introducing a basis set. In order to define the basis set, the given unit cell was divided into non-overlapping, touching spheres called muffin-tin (MT) spheres. The muffin-tin potential is assumed to be spherically symmetric close to the nuclei/core and is assumed to be plane in the interstitial
region. The solutions of the Schrödinger equation outside the MT spheres are plane waves; in this region, the potential is constant. The solutions of the Schrödinger equation inside the MT spheres are made up of angular momentum partial waves. The solutions for the entire space are obtained by matching the two solutions at the boundaries of the MT spheres. The convergence of the combined basis set is controlled by a cutoff parameter $R_{MT} \times K_{max}$, where $R_{MT}$ is the smallest muffin-tin sphere radius in the unit cell and $K_{max}$ is the magnitude of the largest K-vector. Also, the charge leakage from the core is kept minimal. The radii of the muffin-tins employed were 2.6 a.u., 2.6 a.u. and 2.62 a.u. [29] respectively for Dy, Pd and Bi, for the calculations performed initially without spin orbit coupling (SOC) on a k-mesh of 31x31x31 where $RK_{max} = 7$ and $G_{max} = 10$ [30]. Volume optimisation and fitting in equation of states gives the optimised lattice constant as $a_{opt} = 12.5519$ a.u.

In general, the electron’s intrinsic spin couples with its orbital spin angular momentum and give rise to the total angular momentum. All energy levels except for the s-states of one electron atoms are thus split into two substates. This produces the fine structure of the spectral lines. The spin-orbit interaction scales as $Z^2$, hence it is important for atoms with high atomic numbers. For the present f-electron based DyPdBi compound, one has to consider the effect of spin orbit coupling. Accordingly, the above calculations were repeated by including SOC. In both the cases, self consistent field calculations were performed, with an energy convergence of 0.0001 Ryd, and charge convergence of 0.0001 e. Splitting of f-electron bands of dysprosium at the Fermi level is well demonstrated by the Density of States (DoS) histograms that were drawn with SOC (see figure 2). This result ensures the good thermoelectric response of DyPdBi as suggested by G.D.Mahan and J.O. Sofo [26].

In order to explore the band structure of the f-electron based ternary half Heusler compound DyPdBi, the band structure calculation has been extended by performing spin polarized calculations (as DyPdBi is experimentally reported to be magnetic) with Local Spin Density Approximation (LSDA), and with the Perdew-Burke-Ernzerhof (PBE) exchange correlation potential. The spin polarized calculation was performed with a k-mesh of 17x17x17. $RK_{max} = 7$ and $G_{max} = 14$ were used. The radii of the muffin-tin orbitals were 2.5 a.u. for Dy, 2.55 a.u. for Pd, and 2.6 a.u. for Bi. In this case also, self consistent calculations were carried out with the energy convergence of 0.0001 Ry and charge convergence of 0.0001 e. The
optimized lattice parameter was calculated for each of the above mentioned exchange correlation schemes by fitting the volume optimization into the Birch-Murnaghan equation of state. The optimised lattice parameter ($a_{\text{opt}}$), total energy ($E_{\text{tot}}$), Fermi energy ($E_F$), bulk modulus ($B$), density of states at Fermi level ($N(E_F)$) of both the spin-up and spin-down states and spin magnetic moment/unit cell ($\mu_B$) values of DyPdBi compound, by LSDA and PBE correlation schemes, are presented in table 1. The present compound DyPdBi is comprised of dysprosium (Dy) which has half filled f orbitals and is strongly correlated. The behaviour of electrons in such systems can be described well by including the onsite Coulomb interaction in the conventional Hamiltonian. Hence the calculations were done by including the Hubbard potential for dysprosium. The Hubbard potential explicitly includes the Coulomb parameter ($U$) and Coulomb exchange parameter $J$ for the 4f electrons. The value of the Hubbard potential for dysprosium is based upon the literature [31] with $U=0.49$ Ryd and $J=0.05$ Ryd. Coulomb-corrected local spin density approximation (LSDA + U) was applied, as this method, introduced by Anisimov, et al [32], is found to be very efficient for several rare-earth compounds [33, 34, 35, 36, 37, 38, 39].

3. Results and Discussion

3.1. Structural, Electronic and Magnetic properties of DyPdBi

From table 1, it is clear that LSDA underestimates the experimental lattice parameter of DyPdBi whereas the PBE calculation overestimates the same. Due to this, there is considerable shift in the Fermi energy level and fluctuation in the bulk modulus values of the respective scheme. The density of states at the Fermi energy level is very low for the spin-up states in comparison to that for the spin down states. The spin magnetic moment per unit cell ranges between 4.73 $\mu_B$ and 4.87 $\mu_B$.

3.1.1. Density of States (DoS)

The total and partial density of states histograms of DyPdBi as calculated for PBEsol without spin orbit coupling are shown in figures 1(a) and 1(b). From figure 1(a), one finds that the total DoS of the compound DyPdBi is around 110 states/eV at the Fermi energy level, of which around 90 states/eV are contributed mainly by dysprosium. Figure 1(b) suggests that it is only the Dy-f states that contribute to the total DoS of the compound. Thus, nearly 80% of the total DoS at Fermi level is due to Dy-f states alone.
The total and partial density of states histograms of DyPdBi for PBEsol with spin orbit coupling are presented in figures 2(a) and 2(b). From these figures, one can clearly see that the Dy-f states split into two levels; one level comprised of a few states below the Fermi level and the other comprised of a few states at the Fermi level. The states below the Fermi level are shifted down by 1.0 eV from the Fermi level. Figure 2(b) shows that the total DoS at the Fermi level is nearly 54 states/eV, of which 45 states/eV are contributed by Dy-f states. Comparison of figures 1 and 2 suggest that the inclusion of spin orbit coupling in this calculation has reduced the influence of Dy-f states by approximately 50% at the Fermi level besides the splitting that is caused.

Though we performed spin polarised calculations for various exchange correlation schemes, viz., Local Spin Density Approximation (LSDA), PBE and (LSDA + U) on DyPdBi, the DoS histograms are analyzed for LSDA and (LSDA + U) alone as these methods are known to be rather efficient for many of the rare-earth compounds. Figures 3(a) and 3(b) show the total and partial DoS histograms of DyPdBi using LSDA for spin-up and spin-down states respectively. Similarly figures 4(a) and 4(b) show the same for (LSDA+U). From figures 3(a) and 4(a), drawn for spin-up states, it is clear that the total, and hence the partial, DoS is very low of the order of 3-4 states/eV at the Fermi energy level. Inclusion of the Hubbard potential is not of much significance at the Fermi level for spin up states. From figures 3(b) and 4(b), drawn for spin-down states, it can be inferred that the total DoS at the Fermi energy level is almost all due to dysprosium and has increased from 26 states/eV to 30 states/eV. The inclusion of the Hubbard potential did not have much influence on the DoS of dysprosium at the Fermi energy level.

3.1.2. Band Structure

Electronic structure plays a major role in understanding the properties of a given material under ambient conditions. The band structure of the compound DyPdBi is shown in figures 5(a) and 5(b) without SOC, and with SOC, respectively. From figure 5(a), one can infer that without SOC the f-states of dysprosium spread around the Fermi level, making the compound more metallic.

With the inclusion of SOC, from figure 5(b), it is observed that at the Γ point the f-states of dysprosium undergo splitting. The splitting is not as significant for the k-points that run from L-W and X-K points.
Figures 6(a) and 6(b) represent the band structure of spin-up states of DyPdBi for LSDA and (LSDA + U). Analysis of figure 6 shows that the spin-up energy bands of both LSDA and (LSDA+U) have a very narrow peak at the Γ point and above the Fermi level, and the gap between adjacent bands comparatively increases in the LSDA+U calculation. This again depicts the metallic nature of DyPdBi. Mahan [26] has reported that the f-electron states which are more tightly bound in atoms bind little in solids and as a result they give larger contributions to the density of states which are of Lorentzian shape with rather narrow widths. In the present case of DyPdBi also, the spin-up states band structure displays such a narrow peak at the Fermi energy level. The existence of such a Lorentzian narrow peak with a sharp singularity close to the Fermi level is a signature for a potential thermoelectric material. The Lorentzian peak near the Fermi level enhances the electrical conductivity in spin up states.

In contrast, the spin-down energy bands of LSDA and (LSDA+U) shown in figures 7(a) and 7(b) are flat, and they spread just above and below the Fermi level. Further, one can see that the conduction band minimum lies almost along the Fermi energy level except in the vicinity of the Γ point, but the valence band maximum lies just below the Fermi level at about 0.2eV at the Γ point, showing semiconducting-like nature. The presence of such flat bands at the valence band maximum corresponds to a large effective mass and is another key factor to improve the thermoelectric efficiency [40]. Thereby it is inferred that DyPdBi could be semimetallic since it exhibits metallic nature for spin-up band structure calculations, and semi-conducting like behaviour for spin-down calculations.

3.2. Transport Properties

The transport properties of DyPdBi were calculated by using the BoltzTraP code [27] interfaced to the Wien2k program. For background, we refer to the description of Rameshe, et al [40]: The calculations are based on a semi-classical treatment for the solution of the Boltzmann equation utilizing the relaxation time approximation and the rigid body approximation. The Seebeck Coefficient (S), as a function of temperature (T) and doping (ρ), is given by

\[ S(T, \rho) = \frac{\int dE \sigma(E)(E - \mu) df/dE}{\int dE \sigma(E) df/dE} \]
where $f$ is the Fermi function and $\mu$ is the chemical potential. Here $\sigma(E)$ is the transport function given by

$$\sigma(E) = N(E) V^2(E) \tau(E)$$

where $N(E)$ is the density of states, $V(E)$ is the band velocity and $\tau(E)$ is the scattering time. Under the constant scattering time approximation $\tau(E)$ is independent of energy $[41]$. The thermoelectric power factor $S^2\sigma$ is determined by the term $\sigma(T)$ which is given by

$$\sigma(T) = \int dE \sigma(E) \frac{df}{dE}.$$  

The transport properties of DyPdBi based on PBEsol-GGA without SOC, with SOC and with (LSDA + U) calculations were estimated by applying the BoltzTraP code. The values of Seebeck coefficient, power factor, resistivity $\rho$, $\sigma/\tau$ and $S^2\sigma/\tau$ at 300K for Fermi energy thus calculated are listed in table 2. Analysis of this table shows that there is good agreement of our theoretical results with the available experimental data $[15]$ which give the Seebeck coefficient of 92 $\mu$V/K, power factor of 20 $\mu$ Wcm$^{-1}$ K$^{-2}$ and the resistivity of 422 $\mu$Ω -cm. The Boltztrap output that has been calculated for the scheme with SOC at 300K for Fermi energy gives the Seebeck coefficient value to be 138 $\mu$V/Kelvin and the power factor to be 30.8 $\mu$ Wcm$^{-1}$ K$^{-2}$. The estimated power factor value matches well with that of existing potential thermoelectric materials, namely TiCoSb $[30]$ based alloys, that have a maximum power factor of 23 $\mu$ Wcm$^{-1}$ K$^{-2}$ at 850K and 34 $\mu$ Wcm$^{-1}$ K$^{-2}$ for ZrNiSn based alloys $[30]$. The obtained Seebeck coefficient value matches well with that of yet another potential TE material, namely Fe$_2$VAl $[42]$, whose Seebeck coefficient is -130 $\mu$V/Kelvin at 300K.

In order to look for the experimental positive Seebeck coefficient value, graphs are drawn and are explained below. The variation of Seebeck coefficient, $S^2\sigma/\tau$ values, with the total energy is plotted for PBEsol-GGA without SOC, with SOC, and with (LSDA + U) - spin down at temperatures 200K, 300K and 400K. These plots are presented in figures 8 and 9. In these figures, the reference level at zero represents the Fermi energy level in eV and the relaxation time is taken as 0.8x10$^{-14}$ second as suggested in the BoltzTraP user manual. Analysis of figures 8(a)-8(c) reveals a peak in the Seebeck coefficient value and it remains positive just below the Fermi energy for temperatures 200K, 300K and 400K. This is in accordance with the reported literature $[15]$. 

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that suggests the possibility that holes play a major role in the electrical and heat transport properties of the DyPdBi compound. Further, in figure 8(a), we see that the Seebeck coefficient is maximum at 200K and decreases with increases in temperature, whereas in figures 8(b) and 8(c), it remains stable with temperature.

$S^2\sigma/\tau$ is another important parameter to characterize a thermoelectric material as found by the research group of Dresselhaus and others [43, 44, 45]. Its variation with energy for DyPdBi at temperatures 200K, 300K and 400K is shown in figures 9(a), 9(b) and 9(c). One can find two peaks in figure 9(a), one below the Fermi energy level and the other almost at the Fermi energy level. The value of $S^2\sigma/\tau$ is maximum at 400K for both the peaks and is found to decrease with a decrease in temperature. The same observation is seen in figures 9(b) and 9(c), except that there is an additional peak in the case of the scheme drawn with SOC, where the peak lies deep inside the Fermi level.

4. Conclusions

The first principles calculation of the half Heusler DyPdBi compound is investigated and presented by using the full potential - linear augmented plane wave (FP-LAPW) method as implemented in the Wien2k code. Different exchange correlation potentials, namely PBEsol with and without spin orbit coupling, spin polarised LSDA, and LSDA+U were employed. The optimised structural parameter of $a_{opt} = 12.41414a.u.$ was obtained by using LSDA+U and it matches well with the experimental data. Spin polarised calculations reveal that the density of states at the Fermi energy level is greater for spin-down states; it is very feeble for spin-up states. The spin magnetic moment per unit cell ranges from 4.73 to 4.87 $\mu_B$ in the above study. The density of states histogram drawn for PBEsol with spin orbit coupling reveals the splitting of dysprosium f-states at the Fermi energy level. This is to be appreciated, as it is one of the requirements for being a good thermoelectric material. There is approximately a 50 % reduction in the density of states of Dy f-electron states at the Fermi level by the inclusion of spin orbit coupling. The inclusion of onsite coulomb interaction LSDA+U increases the total DoS at the Fermi energy level to 30 states/eV from 25 states/eV. The band structure of spin polarised LSDA+U calculations both for spin-up and spin-down states augments the possibility of DyPdBi to be a potential candidate for TE applications. The band structure of spin-up states reveals the presence
of a Lorentzian narrow peak with a sharp singularity very close to the Fermi level, which is a signature for a potential thermoelectric material. Further, for spin-down states, the presence of localised flat bands that correspond to infinite effective mass at the valence band maximum is another key factor to improve the thermoelectric efficiency.

The calculated power factor $30.8 \mu Wcm^{-1}K^{-2}$ using PBEsol with SOC, and $34.76 \mu Wcm^{-1}K^{-2}$ by LSDA+U, at Fermi energy for 300K are in good agreement with the experimentally reported values.

The above band profile investigations on DyPdBi suggest that it may serve as a good thermoelectric material. Further its efficiency can be improved by doping which allows one to tune the band structure of DyPdBi suitably in order to obtain maximum TE efficiency.

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Table 1. Structural, Electronic and Magnetic properties of DyPdBi

| Parameter                          | Spin Polarised                      |
|------------------------------------|-------------------------------------|
|                                    | LSDA | PBE | (LSDA+U) |
| Lattice Parameter (a.u)            |      |     |          |
| $a_{expt} = 12.53884$ [15]         |      |     |          |
| $a_{opt} = 12.3808$                |      |     |          |
| $a_{opt} = 12.7472$                |      |     |          |
| $a_{opt} = 12.4114$                |      |     |          |
| $E_F$ (Ryd)                        | 0.534 | 0.4855 | 0.5429 |
| $E_{tot}$ (Ryd)                    | -77545.867563 | -77594.12155 | -77545.76333 |
| B (GPa)                            | 115.4130 | 70.2516 | 88.6747 |
| $N(E_F)^\uparrow$/Ryd             | 3.02 | 3.71 | 4.64 |
| $N(E_F)^\downarrow$/Ryd           | 482.56 | 178.30 | 584.80 |
| Spin Magnetic moment per unit cell ($\mu_B$) | 4.87 | 4.83 | 4.73 |
Table 2. Transport Properties of DyPdBi at 300 K for Fermi Energy

| Method                        | Seebeck Coefficient (S) ($\mu$V/K) | Resistivity ($\rho$) ($\mu$Ω-cm) | $\sigma/\tau \times 10^{19} (\Omega^{-1} m^{-1} s^{-1})$ | $S^2 \sigma/\tau \times 10^{14} (\mu W cm^{-1} K^{-2} s^{-1})$ | Power Factor ($\mu W cm^{-1} K^{-2}$) |
|-------------------------------|------------------------------------|-----------------------------------|------------------------------------------------------------|-----------------------------------------------------------------|---------------------------------------|
| Without SOC                   | -107.1                             | 381.381                           | 3.28                                                       | 37.6                                                             | 30.09                                 |
| With SOC                      | -138                               | 618.465                           | 1.04                                                       | 19.8                                                             | 30.81                                 |
| (LSDA+U) for spin down        | -113                               | 370.547                           | 3.38                                                       | 43.5                                                             | 34.76                                 |
| (LSDA+U) for spin up          | 8.61                               | 55.306                            | 22.6                                                       | 1.674                                                             | 1.339                                 |
Figure 1. (a) Total and (b) partial DoS histograms of DyPdBi without SOC.
Figure 2. (a) Total and (b) partial DoS histograms of DyPdBi with SOC.
Figure 3. DoS histograms for (a) spin up and (b) spin down states of DyPdBi by LSDA.
Figure 4. DoS histograms for (a) spin up and (b) spin down states of DyPdBi by (LSDA+U).
Figure 5. Band structure of DyPdBi drawn (a) without SOC and (b) with SOC.
Figure 6. Band structure of spin-up states of DyPdBi (a) for LSDA and (b) for (LSDA+U).
Figure 7. Band structure of spin-down states of DyPdBi (a) for LSDA and (b) for (LSDA+U).
Figure 8. DyPdBi Seebeck Coefficient vs total energy.
Figure 9. DyPdBi $S^2\sigma/\tau$ vs total energy.