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Contents

A Theoretical Investigation of Superconductivity & Electronic Structure of AlB_2 and BeB_2

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Abstract

Superconducting state parameters of AlB_2 and BeB_2 have been theoretically estimated by employing Ashcroft potential [Phys.Lett. 23, 48(1966)] and R.P.A. form of dielectric screening due to Linhard [Kgl.Danske Videnskab. Selskab, Mat-fys. Medd. 28, 8 (1954)] in BCS-Eliashberg-McMillan framework. The present investigations provide T_C value for BeB_2 in good agreement with the experimental data due to Yang et al. [cond-mat/0104063 (2001)]. The T_C value of AlB_2 is also found to be in good agreement with the other theoretical results due to Bohnen et al. [cond-mat/0103319 (2001)]. In order to further investigate the issue, the band structure and density of states of these compounds have also been computed from Density Functional theory by employing generalized gradient approximation. On comparison with relevant diagrams for MgB_2, it may be concluded that BeB_2 stands good chances to become a super conductor whereas the electronic structure studies of AlB_2 show less probability of it to become a superconductor. The present findings thus strongly support possibility of experimentally observing superconductivity in BeB_2 whereas AlB_2 stands less chances to become a superconductor.

Keywords. *Superconductivity; pseudopotential; transition temperature; electron-phonon interaction; metallic diborides; electronic structure; band structure; density of states*

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1. Introduction

The discovery of superconductivity in MgB_2 at 39k by Nagamatsu et al in 2001[1] created interest in other metallic and transition metal diborides leading to several experimental and theoretical researches on these compounds. Superconductivity was discovered in NbB_2 with T_C = 3.87K thirty one years earlier to MgB_2 by Cooper et al.[2]. Leyarovska et al.[3] experimentally investigated metallic and transition metal Diborides MB_2 (M = Li; Be, Al, Ti, Zr, Hf, V, Nb, Ta Cr, Mo) down to 0.42 K and had showed as early as in 1979 that only NbB_2 of these show superconductivity at T_C = 0.62K. They did not check MgB_2. Kaczorowski et al.[4] observed superconducting transition in TaB_2 at T_C = 9.5 K, but they could not observe superconductivity in TiB_2, HfB_2, VB_2, NbB_2 and ZrB_2. Although according to Felner[5] BeB_2 does not superconduct, but Young et al.[6] observed that $BeB_{2.75}$ is a superconductor with T_C ~ 0.7 K. Gasparov et al.[7] found ZrB_2 to superconduct at T_C = 5.5 K, but they could not observe superconductivity in TaB_2 and NbB_2.

Bohnen et al.[8] theoretical investigated superconductivity and phonon dispersion in MgB_2 and AlB_2 by using a mixed-basis pseudo-potential method in density functional perturbation theory. The values of electron-phonon coupling strength (λ) for the two borides obtained by them were $\lambda_{MgB2} = 0.73$ and $\lambda_{AlB2} = 0.43$. For Coulomb pseudopotential they take $\mu^* = 0.05$ to obtain $(T_C)_{MgB2} = 40K$ and $(T_C)_{AlB2} \sim 9K$. By employing a similar approach Heid et al.[9] investigated transition metal diborides like TaB_2, VB_2, NbB_2, TiB_2 and YB_2 along with MgB_2 and AlB_2. They obtain same values of λ for MgB_2 and AlB_2 as obtained by Bohnen et al.[8], but on using $\mu^* = 0.13$ they obtain $(T_C)_{MgB2} = 21.7$ K and $(T_C)_{AlB2} = 2.3K$. They find λ and logarithmic phonon frequency (ω_{log}) values to be most favourable for MgB_2 to be a superconductor. Their investigations show all the above mentioned transition metal diborides to be superconducting, except for TiB_2.

Bester and Fähnle[10] investigating covalent bond energies observe that both in MgB_2 and AlB_2 there is a metallic contribution to the bonding between the layers which is stronger for Al than for Mg. Medvedeva et al.[11] investigate band structure of CaB_2, BeB_2, AlB_2, ScB_2 and YB_2 in comparison with that of MgB_2 and on that basis they explain the absence of medium -T_C superconductivity in BeB_2, AlB_2, ScB_2 and YB_2. Experiments conducted by Methfessel and Scheffler[12] also provide similar result for BeB_2. For AlB_2 Medvedeva et al.[11] observe that p_{xy} – bands are completely filled up and therefore AlB_2 is not a superconductor.

Satta et al.[13], on the basis of electronic structure calculations performed by them, observe that as compared to MgB_2, BeB_2 has similar filling of σ bands, but differs in terms of π states near E_F. The density of states at E_F is lower and E_{2g} phonon frequency is substantially higher in BeB_2, while other phonon frequencies are comparable or lower than MgB_2. However, they do not provide a conclusive result for BeB_2 to be superconducting or not.

Neaton and Perali[14] have determined the density of states at Fermi level, N(0), for CaB_2, NaB_2 and AlB_2. The values obtained by them for the three metallic borides were 0.981, 1.014 and 0.378 states / eV-cell respectively, the relevant value for MgB_2 being 0.711 states / eV-cell. On the basis of large increase in N(0) for CaB_2 and NaB_2, they obtain T_C values of 65.6K and 68.5K respectively. But for expanded c-axis the stability of the two borides is in question. The low value of N(0) for AlB_2 makes it less favourable to become a superconductor.

Known et al.[15] on the basis of electronic structure calculations in AgB_2 and AuB_2 observe that B_{2p} density of states dominate at Fermi level in comparison with Ag-4d and Au-5d states and λ-values for AgB_2 (=1.35) and AuB_2 (=1.65) are much higher than for MgB_2 (=0.79). The estimated T_C values being 59K for AgB_2 and 72K for AuB_2, as compared to the calculated $T_C = 27K$ for MgB_2. Similarly for CuB_2 they report $\lambda = 1.48$ and $T_C = 65K$. However, experimental verification of these results is still awaited.

Singh[16] has investigated electron-phonon interaction in NbB_2 and MgB_2 and obtained λvalues to be 0.43 and 0.59 respectively for these compounds, which provide T_C values around 3K for NbB_2 and 22K for MgB_2. Mehl et al.[17] on the basis of density functional calculations show CuB_2 to be a superconductor with $\lambda = 0.86$ and $T_C = 48K$, as compared to $\lambda = 0.78$ and $T_C = 38K$ obtained by them for MgB_2. As such, there exists a state of uncertainty regarding superconducting behaviour of metallic borides other than MgB_2, requiring reinvestigation of metallic and transition metal diborides.

Recently Sharma et al.[18] have successfully explained superconducting state properties of MgB_2 by employing a pseudopotential approach in BCS-Eliashberg-McMillan framework, obtaining $\lambda = 1.058$, $\mu^* = 0.124$ and $T_C = 39.27$ K.

In the present work we extend the methodology used by Sharma et al.[18] for investigating superconductivity in two metallic diborides BeB_2 and AlB_2. Be being in the same group as Mg and situated just above it and Al being in the same row as Mg and situated immediately next to it in the periodic table, their borides are expected to share some common features with MgB_2. The most important property of MgB_2 is its medium T_C superconductivity. As such, we expect BeB_2 and AlB_2 also to show superconductivity, may be at lower temperatures, because all these three borides have identical crystallographic structure of AlB_2 (C32), which is hexagonal, space group P6mmm with graphitic B-planes and 12 fold B-coordinated Al atoms sitting at the center of B hexagonal prisms. The unit cell contains one formula unit, with Al atom at the origin of the coordinates and two B atoms in positions:

$$\vec{r}_1 = \left(\frac{a}{2}, \frac{a}{2\sqrt{2}}, \frac{c}{2}\right) \text{ and } \vec{r}_2 = -\vec{r}_1$$

In the present investigations we use Ashcroft's potential[19] and R.P.A. form of dielectric screening due to Linhard[20], which have been found to work well in explaining superconductivity in metallic glasses by Sharma et al.[21].

In order to further investigate the electronic structure of these metallic diborides, we determine their band structure and density of states by using generalized gradient approximation[22] in Density Functional theory[23]. For this purpose we employ WIEN 2K10 Code due to Schwarz et al.[24].

2. Theory

In BCS-Eliashberg-McMillan Formulation the electron-phonon coupling strength is given by[25]

(2.1) $$\lambda = 2\int_0^\infty d\omega\left[\alpha^2(\omega)F(\omega)/\omega\right]$$

Here $\alpha^2(\omega)F(\omega)$ is the spectral function which, when appropriately evaluated in the plane-wave approximation for scattering on the Fermi surface, gives

(2.2) $$\lambda = \frac{12 m_b z}{M<\omega^2>}\int_0^1 dx\, x^3 |v_s(x)|^2$$

where $\vec{x} = \vec{q}/2k_F$, $\vec{q}$ being the momentum transfer in scattering on the Fermi surface from state $|\vec{k}>$ to state $|\vec{k}+\vec{q}>$ and k_F is the Fermi radius. Here m_b represents the band mass of the electron, M is the ionic mass averaged on the formula unit of the crystalline compound, z being its effective valence, $<\square^2>$ the average square phonon frequency of the compound and $v_s(x)$ represents the screened pseudopotential form factors at the Fermi surface.

For estimating $<\omega^2>$ we follow known et al.[15], in writing :

(2.3) $$<\omega^2> = \frac{1}{2}\theta_D^2$$

where θ_D is the Debye Temperature of the compound or alloy under consideration. The Coulomb repulsion between the electrons in a superconductor is estimated by the Coulomb pseudo potential (μ^*) given by Morel and Anderson in the following form[26] :

(2.4) $$\mu^* = \frac{\frac{m_b}{\pi k_F}\int_0^1 \frac{dx}{x\in(x)}}{1+\frac{m_b}{\pi k_F}\ln\left(\frac{k_F^2}{20\theta_D}\right)\int_0^1 \frac{dx}{x\in(x)}}$$

where $\in(x)$ is the dielectric screening function and k_F is the Fermi radius. After evaluation of λ and μ^* from equations (2.2) and (2.4) respectively, the estimation of transition temperature (T_C) and isotope effect exponent (α) can be made in a straight forward manner by employing the relevant expressions due to McMillan[25] :

(2.5) $$T_C = \frac{\theta_D}{1.45}\exp\left[\frac{-1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right]$$

and

(2.6) $$\alpha = \frac{1}{2}\left[1-\left(\mu^*\ln\frac{\theta_D}{1.45T_C}\right)^2\frac{1+0.62\lambda}{1.04(1+\lambda)}\right]$$

For interaction strength (N_0V) we follow Rajput & Gupta, in writing[27] :

$$N_e V = \frac{\lambda - \mu^*}{1 + \left(\frac{10}{11}\right)\lambda}$$

The relevant expressions for Ashcroft's empty core model pseudopotential[19] and RPA form of dielectric screening[20] used in this work are given by:

$$v_{(x)} = \frac{-\pi z^*}{\Omega_0 x^2 k_F^2} \cos(2x k_F r_c)$$

and

$$\epsilon(x) = 1 + \frac{m^*}{\pi k_F x^2}\left[0.5 + \frac{(1-x^2)}{4x} \ln\left|\frac{1+x}{1-x}\right|\right]$$

where z^* is the effective valence of the electron given by

$$z^* = (2\text{-}m_E)z$$

m_E being the component of effective mass (m^*) of the electron taking care of non-locality in energy, Ω_0 is the atomic volume and r_c is the potential parameter.

3. Results and Discussion

In the present investigations we treat the metallic diborides by pseudo-atom formalism, in which the component atoms are replaced by pseudo atoms with average properties. In this model the potential parameter r_c is treated as a fitting parameter and other input parameters are obtained from the relevant values of component metals by using the Vegard's rule[21].

The values of input parameters thus obtained for BeB_2 and MgB_2 have been assembled in Table 1.

Table 1 : Input parameters

Parameters	AlB_2	BeB_2	MgB_2
m_h	1.04	1.036	1.03
m_E	0.94	0.97	0.933
m^*	1.426	1.356	1.3727
M(amu)	16.201	10.211	15.311
Ω_0(au)	69.910	50.93	84.7667
k_F(au)	1.1210	1.1547	1.0532
z	3.000	2.667	2.667
$\langle\omega^2\rangle\times10^{-5}(K^2)$	4.7369	6.8056	2.45687
θ_D(K)	973.33	1166.66	700
r_c	1.223	0.999	1.551

The r_c values for the two borides shown in Table 1 are obtained by fitting to the form factors of the compounds obtained from those of component elements by using the Vegard's rule. The relevant form factor curves ($V_x - x$ diagrams) for AlB_2 and BeB_2 are shown respectively in Figures 1 and 2.

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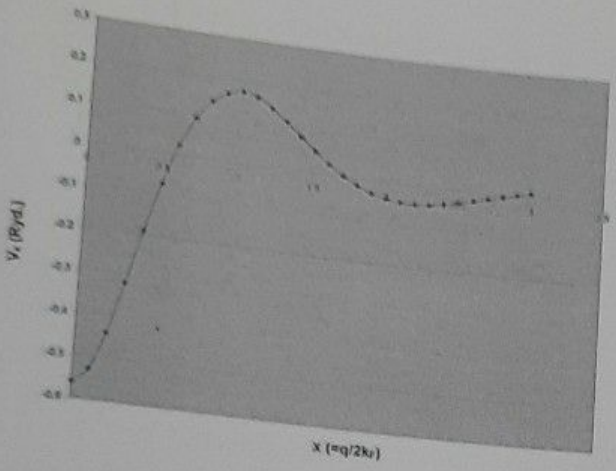

Figure 1. Form factors of AlB_2

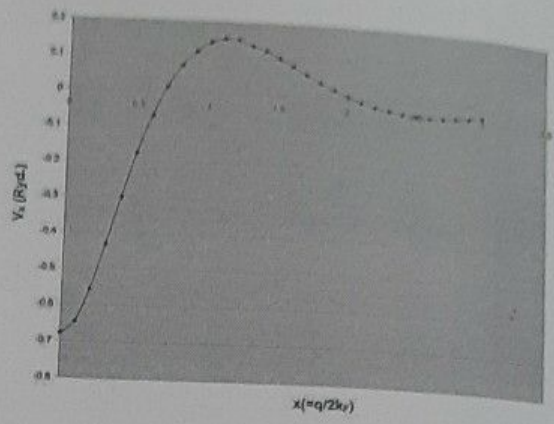

Figure 2. Form factors of BeB_2

The values of superconducting state parameters of the two compounds obtained from the present investigations are assembled in Table 2, where we also include relevant results for MgB_2, rederived from the present formulation, for the sake of comparison.

Table 2 : Superconducting state parameters of metallic borides

Alloys	λ	μ^*	$(T_C)_{Calc}$ (K)	$(T_C)_{Exp.}$ (K)	α	N_0V
AlB_2	0.5351	0.1235	9.03	9.0[a], 2.3[b]	0.38	0.28
BeB_2	0.3550	0.1262	0.72	0.7[c]	0.16	0.17
MgB_2	1.0573	0.1236	39.26	39.0[d], 39.2[e]	0.46	0.48

a : Bohnen et al. [8]; b : Heid et al. [9]-theoretical result;
c : Young et al. [6]; d : Nagamatsu et al. [1]; e : Osborn et al. [28] – experimental results.

It may be observed from Table 2 that whereas the present results for MgB_2 are in excellent agreement with the values reported earlier by Sharma et al.[18], the present results for AlB_2 are in good agreement with the results of Bohnen et al.[8]. The present value $\lambda = 0.5351$ for AlB_2 is quite close to $\lambda_{AlB2} = 0.43$ obtained by Bohnen et al.[8], but they used $\mu^* = 0.05$ empirically, whereas we have derived $\mu^* = 0.1235$ from fundamental considerations from R.P.A. screening, which is more realistic. The present value of T_C for AlB_2 (9.03K) is in excellent agreement with the value 9.0K reported by Bohnen et al.[8]. μ^* (=0.13) used by Heid et al.[9] for AlB_2 was close to our value (μ^*=0.1235), but their value of T_C(=2.3 k) was lower in magnitude than the present value (9.03k) and the value 9.0k reported by Bohnen et al.[8]. Though the present result is in contrast to the experimental situation where no superconductivity has been found so far for AlB_2, but the presently computed value of isotope effect exponent $\alpha = 0.38$ and interaction strength $N_0V = 0.28$ suggest that AlB_2 should show superconductivity, which is supported by the fact that both the component elements (Al and B) are superconductors, with transition temperatures : $(T_C)_{Al} = 1.17$ K (3.6K for films) and $(T_C)_B = 11.2$ K at 250 Gpa (Buzea and Yamashita[29]). The theoretical investigation of Bohnen et al.[8] and Heid et al.[9] support the view, that AlB_2 should show superconductivity.

For BeB_2 we obtain $T_C = 0.72$K, which is in excellent agreement with the experimental value (=0.7K) reported by Young et al.[6]. Though Medvedeva and Ivanovskii[11] and Satta et al.[13] have not been able to find superconductivity in BeB_2, yet Satta et al. have expressed possibility of BeB_2 to be a superconductor on the basis of electron energy bands and phonon frequencies. The present results

showing the presence of isotope effect in BeB_2 with $\alpha = 0.16$, and interaction strength $N_0V = 0.17$ strongly favour it being a superconductor. Small values of α and N_0V suggest that this should be a weak coupling superconductor with comparatively smaller values of λ and T_C. Possibility of superconductivity in BeB_2 is further supported by the fact that both the component elements (Be and B) are superconducting with transition temperatures $(T_C)_{Be} = 0.026K$ (9K for films) and $(T_C)_B = 11.2K$ at 250 Gpa. (Buzea and Yamashita[26]).

The band structure diagram of MgB_2, BeB_2 and AlB_2 as obtained from density functional theory[23] by employing generalized gradient approximation due to Perdew et al.[22] and WIEN 2K10 code due to Schwarz et al.[24] are shown in Figures 3 to 5 and relevant density of states are shown in Figs. 6 to8. It may be observed from the Band structure diagrams of MgB_2 (Fig.3) that the medium temperature superconductivity shown by it may be attributed to the position of p_{x-y} band just above the Fermi level at Γ point and nearly cylindrical structure of the Fermi surface about the ΓA symmetry line. The total density of states (Fig.6) at Fermi level being of the order of 0.71 states / ev creates favorable conditions for pairing of electrons exist in MgB_2. Thus the electronic structure of MgB_2 is very much favorable for it becoming a superconductor at medium temperatures of the order of 40K.

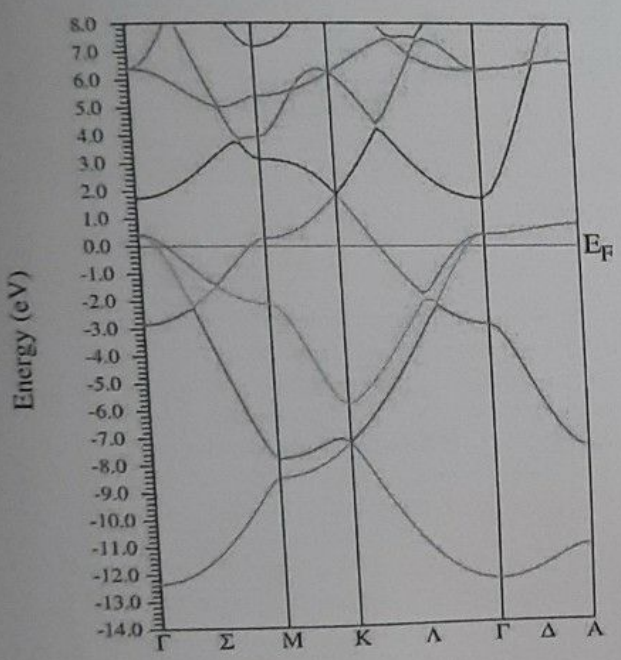

Figure 3. Band structure of MgB_2

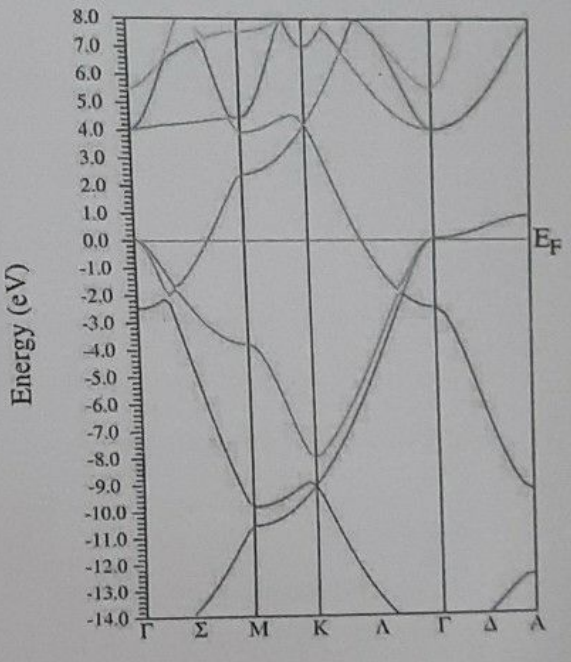

Figure 4. Band structure of BeB_2

The band structure diagram of BeB_2 (Fig.4) reveals that the p_{x-y} band just passes through the Fermi level at Γ point and the Fermi surface around the ΓA symmetry line will form a cone rather than a cylinder. Figure 7 also reveals that the density of states at Fermi level in BeB_2 is of the order of 0.48 states/ev. Thus the electronic structure properties of BeB_2 make it less favourable for superconductivity, as compared to MgB_2. However, they are still quite appropriate for BeB_2 to be a superconductor. The BeB_2 should therefore, become a superconductor at comparatively lower temperatures.

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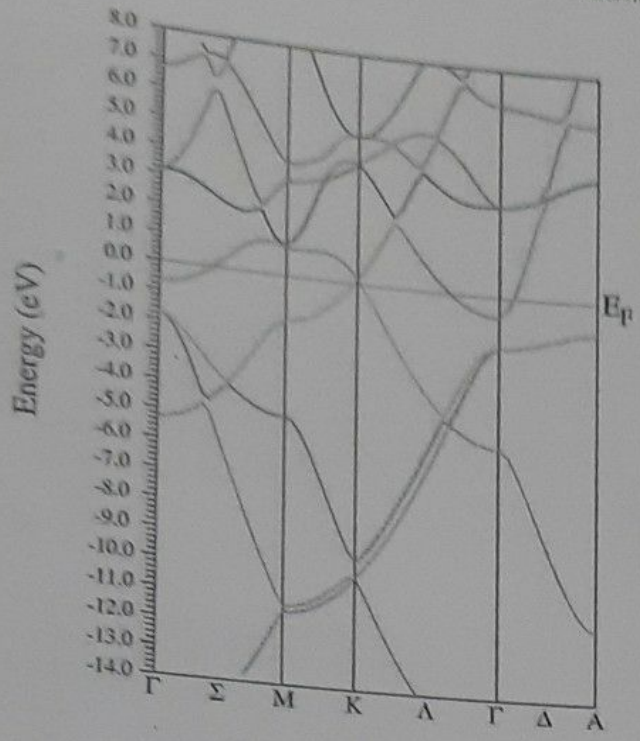

Figure 5. Band Structure of AlB_2

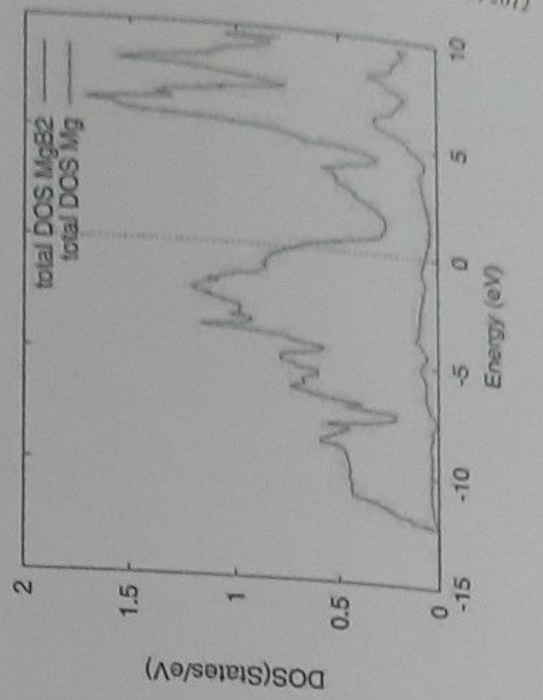

Figure 6. Density of States of MgB_2

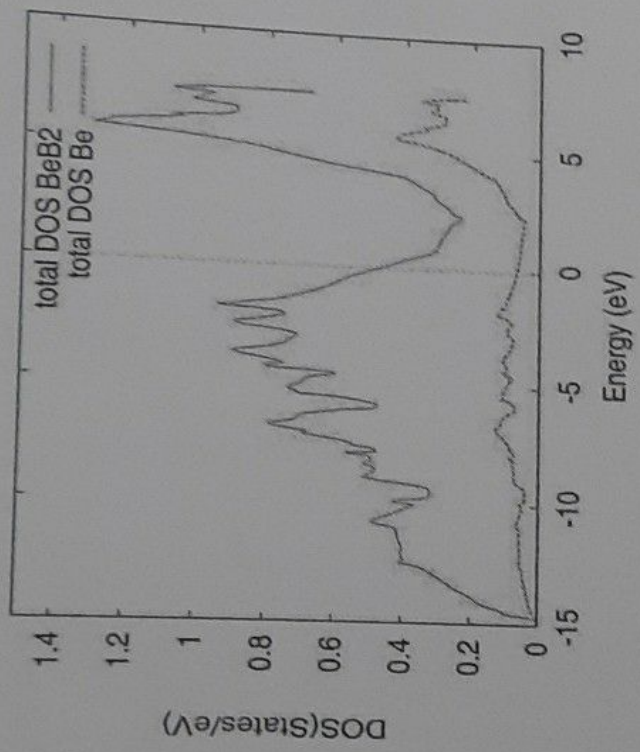

Figure 7. Density of States of BeB_2

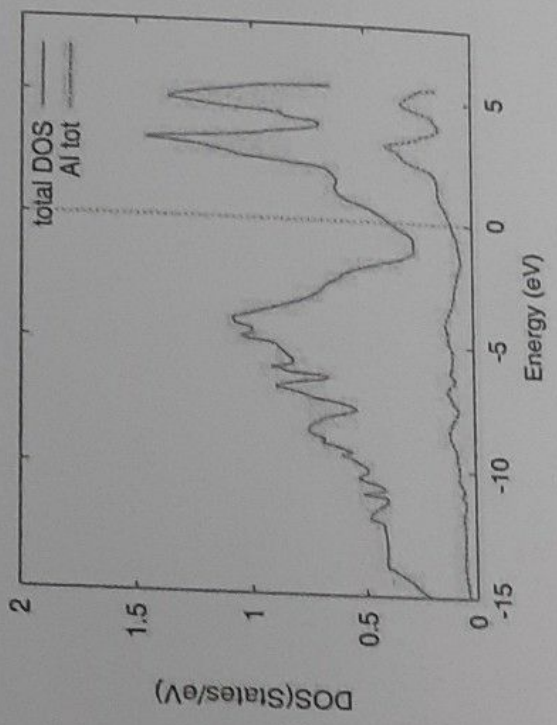

Figure 8. Density of States of AlB_2

A glance at the band structure diagram of AlB_2 (Fig.5) reveals that the p_{xy} band at Γ point lies well below the Fermi level so that all the states in this band are filled up. The density of states of AlB_2 (Fig.8) at Fermi Level (being of the order of 0.38 states/ev) is also much smaller as compared to MgB_2. This makes AlB_2 less favorable to become a superconductor. However, nearly cylindrical Fermi surface about ΓA line in AlB_2 may help in coupling of electrons which creates some possibilities for it to show superconductivity. As such, to sum up we can say that the electronic structure studies strongly support BeB_2 to be super conductor but AlB_2 is less likely to show superconductivity.

4. Conclusions

The present investigations from BCS-Eliashberg McMillan formulation support the possibility of observing superconductivity in both the metallic diborides, AlB_2 and BeB_2. The electronic structure studies i.e. the band structure and density of states obtained from Density Functional Theory also support this result and show that BeB_2 stands better chances than AlB_2 to become superconductor. A systematic experimental study is warranted to check these compounds as well as other metallic and transition metal Diborides for the presence of superconducting state in them, so as to finally settle down the question relating to the presence of superconductivity in this compounds.

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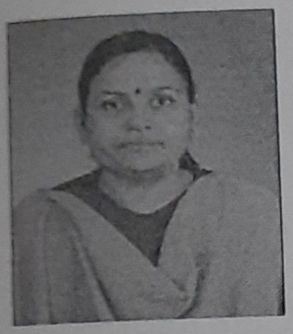

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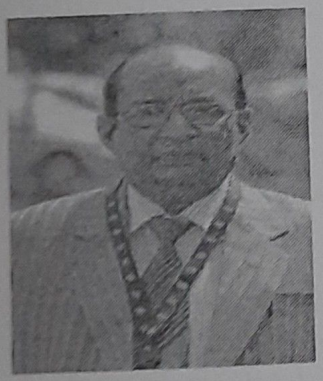

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