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A UNIFIED THEORETICAL APPROACH TO SUPERCONDUCTING STATE PARAMETERS AND ELECTRONIC STRUCTURE OF Mg, B AND MgB_2

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ABSTRACT

Pseudo potential theory has been applied in BCS-Eliashberg-McMillan framework by employing T_c-equation due to Allen and Dynes for estimation of superconducting state parameters, viz., electron-phonon coupling strength (λ), Coulomb pseudo potential (μ^*), transition temperature (T_c), isotope effect exponent (α) and interaction strength (N_oV) of Mg, B and MgB_2 in a unified theoretical approach. For MgB_2 we use form factors obtained from the relevant values of component metals (Model-I), and also from the pseudo-atom model with average properties of atoms and appropriate choice of potential parameter (Model-II). The values of superconducting state parameters of Mg, B and MgB_2 obtained from the two models, are found to be in excellent agreement with the available experimental data and other theoretical results. The explicit dependence of λ and T_c on the isotopic mass of Mg and B, as revealed from the present work, confirms the role of lattice vibrations in the superconducting behaviour of MgB_2 The Electron Energy Bands and Density of States of Mg, B and MgB_2 obtained from Density Functional Theory in Generalized Gradient Approximation, by employing WIEN 2K10 code, are also reported.

Keywords: *Pseudo potential, superconductivity, transition temperature, electron-phonon coupling strength, isotope effect, interaction strength, electronic structure, electron energy bands, electron density of states, density functional theory.*

1. INTRODUCTION

Superconductivity in MgB_2, reported in 2001 by Nagamatsu et al.[1] at about 39K is one of the rare discoveries to cause a great hustle and bustle in the scientific community, which led to a great volume of research on MgB_2 in the past few years. Discovery of a new phase of Boron, orthorhombic γ-B_{28}, synthesized independently by Chen and Solozhenko in 2004, the structure of which was reported by Oganov et al. [2] in 2009 and the observation of superconductivity in Boron by Eremets et al. [3] in 2001 have created renewed interest in Boron as well. Eremets et al. [3] on compressing β-B_{106}, an allotrope of Boron, at room temperature observed metallization at 160Gpa, and the metallic state displayed superconductivity with T_c = 11.2K at 250Gpa. The structure of this phase of Boron (represented by α-Ga) is not yet known.

Mg crystallizes [4] in to hexagonal closed packed (hcp) structure with p63/mmc symmetry (space group no. 194) and lattice parameters as a_o = 3.2094 A°and c_o = 5.2108 A°.

The crystal structure of Boron, on the other hand, depends on its allotropic form. Crystalline Boron has following five major polymorphs, other than the superconducting phase [5-9]:

1. Rhombohedral α-B_{12}: It crystallizes [5] with symmetry R-3mr (space group no. 166). The rhombohedral cell with density =2.46 gcm^{-3} is a distorted cubic packing of icosahedra containing 12 B atoms with cell parameters a_o=5.06A° and the rhombohedral angle a = 58.06°.

2. Rhombohedral β-B_{106}: This phase of Boron, with density = 2.35 gcm^{-3}, also crystallizes [6] in the R-3m space group. The principal base unit of β-B_{106} is a polyhedron B_{84}, in which 12 pentagonal pyramids B_6 surround the icosahedron B_{12}. The packing of the polyhedra is a distorted cubic packing with a_o= 10.17 A°,and α = 65.20° .

3. Orthorhombic γ-B_{28}: This is a recently discovered phase of Boron [2,7], with density 2.52 gcm^{-3}, which crystallizes in the space group Pnnm with orthorhombic syngony a_o= 5.0544 A°, b_o = 5.6199A° and c_o= 6.9873 A°. The structure consists of icosahedra B_{12} and pairs B_2, which are located at points of the distorted lattice of NaCl type. As a result of charge transfer between the two, B_{12} icosahedra play the role of anions and B_2 pairs act as cations.

4. Tetragonal T-B_{192}: This phase (also called as β-tetragonal Boron) crystallizes in the $P4_3m$ space group (tetragonal syngony a_o= 10.14 A° and c_o= 14.17 A°) [8,9] and belongs to the α –AlB_{12} structure type. The density of this phase is 2.36 gcm^{-3}.

5. I-tetragonal T-B_{50}: This phase (also called as a-tetragonal Boron) was discovered in 1943. It is now well established that this instead of being a pure phase of Boron, is a compound of composition $B_{50}C_2$ or $B_{50}N_2$[7,8] . It contains 50 Boron atoms in the unit cell and crystallizes in to space group P42/nnm or P42m (tetragonal syngony). The 50 Boron atoms are distributed among four icosahedra and two individual B atoms, pairing with the impurity atoms.The unit cell dimensions are a_o= 8.75 A° and c_o= 5.06 A° and has a density of 2.31 gcm^{-3}.

MgB_2 crystallizes in to AlB_2 type structure with P6/mmm symmetry (space group no. 191) with lattice parameters a_o= 3.085 A° and c_o= 3.520 A°. It has graphite like layered structure. The boron atoms lie at the corners of hexagons, which form honeycombed layers. The magnesium atoms are located above and below the centres of hexagons in between boron planes.

The electronic structure of MgB_2 is now well understood [10-15]. The Mg atoms in MgB_2 get ionized and the two electrons donated by each of the Mg atoms are transferred to the boron layers resulting in to an ionic compound Mg^{++} $2(B^-)$. The energy states at Fermi level, which are the highest occupied electron states, are mainly α or π bonding boron orbitals. The σ bonding states are confined in the boron planes whereas π bonding states are aligned perpendicular to the boron planes. The σ bonding states couple strongly to the vibration modes of boron planes, as they are located either in attractive or repulsive bonding modes of boron atoms. The π bonding states do not couple so strongly to the vibration modes. Band structure calculations [10-12] show that approximately 30% of the density of states at Fermi energy are due to planar $Bp_{x,y}$ states (σ bonds), giving rise to nearly cylindrical hole like Fermi surfaces of 2D character. The remaining 70% of the density of states originate in Bp_z states (π bonds), which are strongly hybridized with the Mg s- p orbitals, have 3D character and give rise to mostly electron like Fermi surfaces. The Fermi surface of MgB_2, obtained by Kortus etal.[10] and also recently obtained by Souma et al. [16], show nearly cylindrical double surface about Γ-A direction, which is hole like, whereas the remaining parts of the Fermi surface are more complex and show electron like behaviour.

Belashchenko etal. [13] observe that the band structure of MgB_2 is graphite like, with π bands falling deeper as compared to the energy bands of ordinary graphite. These bands posses a typically delocalized metallic nature as opposed to covalent character. The in-plane σ bands retain their 2D covalent character and exhibit a hole- type metallic conductivity. The coexistence of 2D in-plane and 3D interlayer conducting metallic bands is a peculiar feature of MgB_2. An and Pickett [11] compare band structure of MgB_2 with that of graphite. The valence band in MgB_2 along ΓA direction extends above the Fermi level and has vacant states, whereas in graphite it lies well below the Fermi level and has completely filled states. Kortus et al. [10] also show that the Density of States (DOS) of MgB_2 at the Fermi level is about 0.71 states/ev.

Theoretical efforts to explain superconductivity in MgB_2 with T_c as high as 39K may be categorized as : 1) Extension of BCS theory of low temperature superconductors to higher temperature domain, and 2) extension of the theories of high T_c oxide superconductors, to the low temperature domain. In BCS model, the superconductivity in the low temperature domain is considered to be a consequence of electron phonon interaction, responsible for electron pairing and long range Bose-Einstein condensation of cooper pairs [16]. Coupling of electrons through lattice vibrations or phonons in MgB_2 is supported by the presence of isotope effect in it [17-18].

Realizing electron phonon interaction as the cause of superconductivity in MgB_2, variety of explanations have been provided for the high T_c of the order of 40K in it, a few of which are summarized below:

As per Kortus et al. [10], the fortunate combination of strong bonding, reasonable density of states N(0) at the Fermi level and high phonon frequency of B atoms in MgB_2 are responsible for the high transition temperature in this compound. An and Pickett [11] consider MgB_2 to be a conventional BCS strong coupling s-wave electron-phonon pairing superconductor and attribute its high T_c to: (i) hole doping of the covalent σ bonds, arising through the ionic and layered character of MgB_2, (ii) 2D character of σ band density of states and (iii) an ultra-strong deformation potential of the σ bands from the bond stretching modes. Important role played by E_{2g} phonons in electron-phonon interaction was realized by them. Kong et

al.[12] concluded that the unexpected high T_c in MgB_2 is due to the large value of electron-phonon coupling strength (λ) caused by the presence of holes in the B-B bonding σ band and the relative softness of the optical bond stretching modes. They categorize MgB_2 as an intermediate coupling electron-phonon pairing s-wave superconductor. Yildirim et al. [19] observed that a giant anharmonicity in the in-plane boron phonons with E_{2g} symmetry near the zone centre and non linear electron-phonon coupling are the key effects to the quantitative explanation of the observed high T_c and boron isotope effect in MgB_2.

On the basis of inelastic neutron scattering measurements of phonon density of states, Osborn et al. [20] concluded that a conventional phonon mechanism with high frequency phonons and moderately strong electron-phonon coupling can explain the observed superconductivity in MgB_2. Choi et al. [15] attribute high T_c in MgB_2 to the raising effect of anisotropy in electron-phonon coupling and lowering effect of anharmonicity in the relevant phonon modes. Ravindran et al. [21] calculated Debye temperature of MgB_2 from its elastic properties and showed that the phonon frequencies in it are quite large. They conclude that high T_c in MgB_2 can be explained through BCS mechanism only if phonon softening occurs or the phonon-model is highly anisotropic. Bohnen et al. [22] studied lattice dynamics and electron-phonon coupling in MgB_2 and observed that the high frequency in-plane boron vibrations are strongly softened and exhibit an exceptionally strong coupling to electron states at the Fermi energy.

On the other hand Alexandrov [23] observed that the remarkably low value of Fermi Energy (E_F) and the strong coupling of carriers with high frequency phonons is the cause of high T_c in MgB_2, which may be considered to be in the non adiabatic regime like cuprates, where Migdal-Eliashberg theory is inappropriate. Cappelluti et al. [24] also observed that high T_c superconductivity in MgB_2 is mainly driven by the σ band states. The peculiar feature of such bands is the smallness of the Fermi energy, which induces non-adiabatic channels of electron-phonon interaction.

Hirsch and Marsinghlio [25], exploited similarity of planar structure between the Cu-O planes in cuprates and B-planes in MgB_2 and proposed that like cuprates, superconductivity in MgB_2 originates from some novel mechanism in which holes play a dominant role. Electronic structure of MgB_2 is similar to that of graphite, but whereas σ bands in graphite are full, they are partially empty in MgB_2 and create hole type conduction bands, as is also the case with high T_c cuprates. Positive Hall coefficient observed in MgB_2 by Kang et al. [26] supports this hypothesis.

Varshney et al. [27] on the basis of an effective two dimensional dynamic interaction potential, incorporating the screening of holes as carriers by charge density fluctuations and optical phonons, also observe that superconductivity in MgB_2 is due to hole carriers in strong coupling regime.

Existence of two superconducting energy gaps have also been reported [28] in MgB_2, a small gap ranging from 1.5 to 3.5 meV and a large gap ranging from 5.5 to 8.0 meV at low temperatures, which vanish at T_c. The sizes of the two gaps are found to change on different parts of the Fermi surface. Several theoretical models for the two gap superconductivity have been given by different groups, of which the important works are due to Choi et al.[29], and Konsin and Sorkin [30]. It has been emphasized that the larger gap (Δ_1~6.8 meV) leads to the strong coupling of σ bonding states of the in-plane vibrations of B atoms, confined to the cylindrical sheets of Fermi surface, which contributes principally to super-conductivity in MgB_2. On the other hand the π bonding states on the remaining parts of the Fermi surface form much weaker pairs (Δ_2~1.8 meV). This pairing is enhanced by the coupling to the σ bonding states. Chen et al.[31] confirmed the presence of two energy gaps by observing two pair breaking peaks in the Raman spectra of poly crystalline MgB_2. They obtained Δ_1=22 cm^{-1} (2.7 meV) and Δ_2=50 cm^{-1} (6.2 meV) and concluded that a conventional phonon mediated pairing mechanism occurs in the planar boron σ bands and is responsible for the superconductivity in MgB_2.

Floris et al. [32] investigated superconducting properties of MgB_2 from first principles by employing Density Functional Theory and obtained satisfactory results for the Transition temperature, T_c , the two gaps and temperature dependence of specific heat.
Most of the theoretical investigations of superconductivity in MgB_2 using electron-phonon interaction are either based on the solution of Eliashberg gap equations in isotropic/ anisotropic form or by using McMillan's T_c equation [33], either in its original form or in its modified form proposed by Allen and Dynes [34], to obtain electron-phonon coupling strength (λ) from the experimental values of T_c, however there is hardly any work in which the electron-phonon coupling strength (λ) has been quantitatively estimated from the spectral function $\alpha^2(\omega)$ $F(\omega)$ or from the electron-ion interaction expressed in the form of a potential.

In the present study we use the well established pseudo potential methodology based on BCS-Eliashberg-McMillan formulation for the investigation of superconductivity in MgB_2 along with its component elements, i.e., Mg and B,

as no reports of theoretical work on superconductivity in B are available in the literature and application of similar tools for an alloy or compound along with its component elements helps us to understand the complex systems in a simpler way. In this approach material properties like electron-phonon coupling strength (λ) and Coulomb pseudo potential (μ^*) are obtained from the knowledge of electron-ion pseudo potential, dielectric screening and phonon spectrum (which is generally replaced by the use of a most representative phonon frequency or an average phonon frequency $<\omega>$). The super-conducting state properties like transition temperature (T_c), isotope effect exponent (α) and interaction strength (N_0V) are then obtained by using the values of λ, μ^*, average square phonon frequency ($<\omega^2>$) and isotopic mass (M) relevant to the superconductor. This approach has been successfully used for theoretically explaining superconductivity in the alloys and metallic glasses [35-38]. In this work we use Ashcroft's empty core model pseudo potential [39] for the sake of simplicity and R.P.A. form of dielectric screening due to Linhard [40], which takes care of exchange and correlation effects in the electron gas through effective mass (m^*), explicitly involved in this screening. T_c equation due to Allen and Dynes [34] is used in which pre-factor $\theta_D/1.45$ of McMillan's formula [33] is replaced by $\omega_{ln}/1.2$, because of its superiority over the former, as explained in [34], where ω_{ln} is the logarithmic average of phonon frequencies, defined by $\omega_{ln} = <\ln \omega>$.

The Electron Energy Bands (EEB) and Density of States (DOS) play an important role in understanding the electronic structure of materials. We, therefore, investigate EEB and DOS of Mg, B and MgB_2 by employing Density Functional Theory. In the present work, we investigate I-tetragonal phase of boron (T-B_{50}), which has simplest structure in the known polymorphs of Boron. Band structure of α–rhombohedral boron has been determined by Schöttke [41], but the electronic structure of tetragonal boron has not been reported so far in literature. The present work, therefore, reports electronic structure of tetragonal boron (T- B_{50}) for the first time.

2. THEORY

We follow McMillan [33] in defining electron phonon Coupling strength by

$$\lambda = 2\int_0^\infty d\omega \left[\alpha^2(\omega) F(\omega)/\omega\right] \quad (1)$$

where $\alpha^2(\omega)F(\omega)$ is the spectral function, which when appropriately evaluated in the plane-wave approximation for scattering on the Fermi surface, yields [37]:

$$\lambda = \frac{m^*}{4\pi^3 k_F MN <\omega^2>} \int_0^{2k_F} dq\, q^3 \left|V^*(q)\right|^2 \quad (2)$$

where q is the change in electron wave vector K in scattering on the Fermi surface, m^* is the effective mass of the electron, M is the ionic mass, N is the ion number density, k_F is the Fermi radius and $<\omega^2>$ is the average square phonon frequency of the system under consideration, and

$$V^*(q) = <k+q|V|k> / \epsilon(q) \quad (3)$$

represents the screened atomic form factors, where $<k+q|V|k>$ is the matrix element for the electron scattering from state $|k>$ to state $|k+q>$ on the Fermi surface (or bare ion potential) and $\epsilon(q)$ is the dielectric screening function.

On using $x = q/2k_F$ and $N^{-1} = \Omega_0 = 3\pi^2 z^*/k_F^3$, we obtain

$$\lambda = \frac{12 m^* z^*}{M <\omega^2>} \int_0^1 dx\, x^3 \left|V^*(x)\right|^2 \quad (4)$$

where Ω_0 represents atomic volume and z^* is the effective valence of ions, which is related to valency z of the corresponding ions [42] by,

$$z^* = (2 - m_E) z \quad (5)$$

Here m_E is the component of effective mass of the electron, taking in to account the non-locality in energy.

The repulsive interaction between electrons in a superconductor is given by the Coulomb pseudo potential (μ^*), which on representing band mass by m_b and Debye temperature by θ_D, is given [43] by:

$$\mu^* = \frac{\dfrac{m_b}{\pi k_F} \int_0^1 \dfrac{dx}{x\varepsilon(x)}}{\left[1 + \dfrac{m_b}{\pi k_F} \ln\left(\dfrac{k_F^2}{20\theta_D}\right) \int_0^1 \dfrac{dx}{x\varepsilon(x)}\right]} \quad (6)$$

The relevant expression for the transition temperature T_c is given [34] by

$$T_c = \frac{\omega_{ln}}{1.2} \exp\left[\frac{-1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right] \quad (7)$$

where ω_{ln}, the logarithmic average of phonon frequencies, can be obtained [12] from

$$\omega_{ln} = \int_0^\infty ln(\omega/\omega_{ln})\left[\alpha^2(\omega)F(\omega)\right]d\omega \quad (8)$$

The isotope effect exponent α is given [33] by

$$\alpha = \frac{1}{2}\left[1-\left(\mu^* ln\frac{\theta_D}{1.45T_c}\right)^2 \frac{1+0.62\lambda}{1.04(1+\lambda)}\right] \quad (9)$$

and for interaction strength N_0V, we follow Rajput and Gupta [44] in writing

$$N_0V = \frac{\lambda-\mu^*}{1+\frac{10}{11}\lambda} \quad (10)$$

For obtaining screened atomic form factors $V^s(x)$ through Eq. (3), we use empty core model pseudo potential V(x) due to Ashcroft [39] and the dielectric screening function $\epsilon(x)$ obtained in Random Phase Approximation by Linhard [40], which have been found to work well in explaining the superconducting state in binary alloys and metallic glasses [35-37] and are given respectively by

$$V(x) = \langle k+q|V|k\rangle = \frac{-\pi z^*}{\Omega_0 k_F^2 x^2}\cos(2k_F r_c x) \quad (11)$$

$$\epsilon(x) = 1+\frac{m^*}{\pi k_F x^2}\left[0.5+\frac{(1+x)}{4x}\ ln\left|\frac{(1+x)}{(1-x)}\right|\right] \quad (12)$$

where r_c is the potential parameter, which represents effective atomic core radius, such that in r–space V=0 for $r < r_c$ and varies as (1/r) for $r > r_c$. The value of rc for a superconductor is obtained by fitting it to some experimental property of the superconductor.

Form factors for MgB_2 in the present work are obtained from the form factors of component elements Mg and B by employing the relation (Model-I).

$$V^s_{MgB_2} = \tfrac{1}{3}\left[V^s_{Mg} + 2V^s_B\right] \quad (13)$$

The form factors of MgB_2 obtained from Eq. (13) are used in Eq. (4) to obtain λ and after obtaining μ* from Eq. (6), we obtain T_c, α and N_0V for MgB_2 respectively from Eqs. (7), (9) and (10).

Though the Fermi surface of MgB_2 is quite complex [10], the Fermi surfaces of component elements Mg and B are quite close to the spherical shape and as such the methodology of computing form factors of MgB_2 from the form factors of component elements is theoretically justified. Another approach (Model-II) to deal with the superconductivity of binary alloys or metallic glasses or inter-metallic compounds is to implant pseudo atoms with average properties at the atomic sites of component elements in the compensating back ground of electron charge distribution. By fitting potential parameter r_c to some experimental property of the superconductor, we may obtain realistic form factors of the system under consideration, which when used in Eq. (4) provide us the value of electron-phonon coupling strength λ. From the knowledge of so arrived value of λ and the value of μ* obtained from Eq. (6), we may deduce the values of T_c, α and N_0V from Eqs. (7), (9) and (10) respectively. In this model electron scattering may be considered to take place on nearly cylindrical parts of the Fermi surface about Γ–A symmetry lines, in conformity with the planar structure of MgB_2 and major contribution to superconductivity being due to B $p_{x,y}$ orbitals.

3 RESULTS AND DISCUSSION

Phonon frequency has an important role in explaining the behaviour of superconductors through appearance of $\langle\omega^2\rangle$ in the expression of λ For estimation of phonon frequencies responsible for electron-phonon coupling in Mg, B and MgB_2, we use the formulation given by Butler[45]

$$\langle\omega^2\rangle^{1/2} = 0.69\theta_D \quad (14)$$

which has been found to yield appropriate values of electron-phonon coupling strength λ in superconductors.

As apparent from Eq. (14), $\langle\omega^2\rangle$ and hence λ depend on the Debye temperature θ_D. As such, the selection of θ_D is very crucial in theoretical explanation of superconductivity in MgB_2. The experimental values of θ_D based on specific heat measurements, as reported by Ravindran et al. [21] are 750 ± 30K, 746K, 800K and 920K, whereas the theoretical value calculated by them is 1016K. The other reported values of θ_D are : 800K by Vogt et al. [46], 911.9K by Balaselvi et al. [47], 860K by Chen et al. [48], 1050 ± 50K by Bonquet et al. [49], 700K by Known et al. [50], and 776 ± 14K by Kremer et al. [51].

Known et al. [50] consider the experimental value of θ_D ~700K to be quite satisfactory for theoretical explanation of superconductivity in MgB_2. In the computer

simulation made by us we observe that higher values of θ_D give lower values of electron phonon coupling strength λ, resulting in lower values of T_c. The value θ_D = 700K, reported by Known et al. [50] seems to be appropriate for superconductivity in MgB_2 and as such we use this value of θ_D in the present work. Pre factor θ_D /1.45 in T_c equation suggested by McMillan [33] was successfully used for MgB_2 by Sharma et al.[52]. In the present work we use pre factor ω_{ln}/1.2 in the T_c equation (7), suggested by Allen and Dynes [34] as an improvement over McMillan's formulation, which plays an important role in the prediction of T_c values.

The importance of the E_{2g} mode of phonon frequencies for superconductivity in MgB_2 has been predicted by Heid et al.[53], An and Picket[11] and Kotegawa et al.[54]. Yildrim et al. [19] observed that the frequency of E_{2g} mode at Γpoint in the phonon spectra of MgB_2 may be taken for ω_{ln}, which has been estimated 74.5 meV by them, whereas the relevant value determined by Goucharov et al.[55] is 76.87meV. We use in the present work the average of the two values, i.e., 75.685meV, which yields ω_{ln}= 878.31 K. For ω_{ln} of B we follow Kortus et al. [10] and take ω_{ln}=700 K , whereas for Mg the value of ω_{ln} not being readily available in literature, we use pre-factor θ_D/1.45 instead of ω_{ln} /1.2, which is justified in view of the low value of T_c (< 0.017 K) for this metal.

For atomic mass (M) we use average isotopic masses for Mg and B, i.e., 24.312 and 10.811 amu respectively, as given by Halliday and Reisnick [56]. The values of other input parameters used in this work have been assembled along with their sources in Table 1. Since the values of m*, m_b and m_E for B are not available in literature, we use relevant values of Al, which belongs to the same group as B.

In pseudo-atom model (Model-II) the relevant values of parameters for MgB_2, except for r_c and θ_D, are obtained from the values of parameters for Mg and B by using the Vegard's rule [35] in the following form:

$$P_{MgB_2} = \frac{1}{3}\left[P_{Mg} + 2P_B\right] \tag{15}$$

where p represents a parameter. The values of potential parameter r_c for the component metals Mg and B, as well as for MgB_2 in pseudo atom model (Model-II) are obtained by fitting the form factors. For θ_D of MgB_2 we use its experimental value θ_D = 700K [50] for reasons discussed as above. The $\langle\omega^2\rangle$ values for component metals Mg and B shown in Table 1 are also based on Eq.(14).

Table 1: Input parameters

Parameter	Values of Parameters for computation of form factors of MgB_2 from Eq.(13) (Model-I)			Values of parameters in pseudo-atom model (Model-II)
	Mg	B	MgB_2	MgB_2
z	2	3		2.6667
Ω_0(au)	155.9[a]	49.2[a]		84.7667
k_F(au)	0.7242[a]	1.2177[a]		1.0532
r_c(au)	1.608	1.038		1.39
m*	1.33[b]	1.394		1.3727
m_b	1.01[a]	1.04		1.03
m_E	0.92[a]	0.94		0.9333
M(amu)	24.312[c]	10.811[c]	15.311	15.311
θ_D(K)	400[b]	1250[d]	700[e]	700[e]
ω_{ln} (K)	-	700[f]	878.31	878.31
$\langle\omega^2\rangle$ x 10-5 (K^2)	0.76389	7.45985	2.33943	2.33943

a = [42]; b = [57]; c = [56]; d = [68]; e = [50]; f = [10]

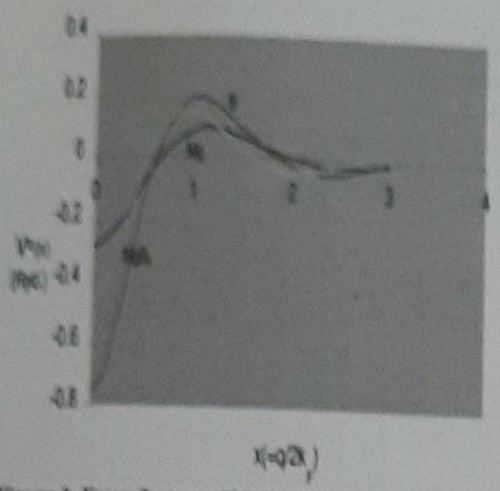

Figure 1. Form factors of MgB_2 obtained from pseudo-atom model (Model-II) along with form factors of component metals (Mg and B)

The form factors of MgB_2 obtained for r_c = 1.39 by using pseudo-atom model (Model-II) are shown in Fig.1, along with the form factors of Mg and B for the sake of comparison.

The values of superconducting state parameters, viz. λ, μ*, T_c, α and N_0V of Mg , using Mc-Millan's T_c equation with pre-factor $\theta_D/1.45$ [33] and for B on using T_c equation due to Allen and Dynes with pre-factor $\omega_{ln}/1.2$ (Eq.7) are displayed in Table 2 along with relevant experimental data and other theoretical results. It may be observed from Table 2 that for Mg, the present values of λ and μ* are in good agreement with the values due to Allen and Cohen [57] and Jain and Kachhava [58] respectively. The present value of T_c for Mg is found to be in good agreement with the experimental value [57] as well as with the values due to Sharma and Sharma [59] and Allen and Cohen [57]. The present value of α (=0.015) is also in good agreement with the value due to Hinks [18], whereas the present value of NoV for Mg (i.e.,0.164) agrees well with the value 0.177 due to Sharma and Sharma [59]. The smaller value of NoV (<0.2) indicates that Mg is a weak coupling superconductor. On the other hand, since there are no other theoretical results of λand μ* for B available in literature, an effective comparison of the present values for these parameters could not been possible. However, an excellent agreement of T_c for B with the experimental values [7, 60] proves the validity of the present results for these parameters. The present value of α for B (=0.382) is in best agreement with the value 0.42 due to Osborn et al. [20]. A comparison of the present value of NoV for B is also not possible due to the absence of other theoretical results, its value (NoV=0.301) suggests that B is a medium coupling superconductor.

Table 2. Superconducting state parameters of Mg and B

Parameters	Values for Mg			Values for B		
	Present	Experimental	Other	Present	Experimental	Other
λ	0.357	-	0.39[a] 0.31[c] 0.35[b]	0.584	-	-
μ*	0.140	-	0.15[a] 0.15[b] 0.14[c]	0.123	-	-
T_c(K)	0.142	< 0.017[b]	0.19[a] 0.08[b] 0.02[c]	11.211	11.2[i]	
α	0.015	-	0.02[d] 0.05[e] 0.08[f] 0.22[f]	0.382	-	0.30[d] 0.46[f] 0.31[e] 0.42[f] 0.28[f]
N_0V	0.164	-	0.18[a] 0.01[g] 0.01[h]	0.301	-	-

a=[59]; b=[57]; c=[58];d=[18]; e=[15]; f=[20]; g=[44]; h=[61]; i=[60]; j=[12]

Table 3. Superconducting state parameters of MgB_2

Parameters	Values obtained from			
	Model I	Model II	Experimental Value	Other Results
λ	0.842	0.842	0.9[a], 0.75[b], 1.4[c], 0.58[d],0.62[e]	0.87[f], 0.79[g], 0.80[h], 0.73[i], 0.87[j], 0.82[k], 0.73[l], 0.61[m], 0.835[n], 0.8408[o], 0.51[p], 1.08[q], 1.40[r], 0.65-1.20[s], 1.40-1.70[t]
μ^*	0.124	0.124	-	0.10[f], 0.10[g], 0.25[i], 0.15[j], 0.10[k], 0.05[l], 0.10[n], 0.13[l], 0.10[o], 0.12[m],0.10-0.14[m], 0-0.2[r], 0.28-0.30[s]
T_c(K)	39.126	39.104	39.0[m], 39.2[a], 39.25[c], 38.5[b], 38.7[e]	27.0[g], 40.0[i], 22.0[p], 21.7[l], 39.0[m], 22.0[g], 40.0[r], 38.75[n], 39.4[o], 39.5[n], 37.0-42.0[m]
α	0.462	0.462	α_B= 0.26[r] α_B= 0.30 & α_{Mg}= 0.02[r]	α=0.21[i], α=0.355[n], α_B=0.30[g], α=0.30[h], α_B=0.46[f], α_B=0.31 & α_{Mg}=0.05[m], α_B=0.42 & α_{Mg}=0.08[n], α_B=0.28 & α_{Mg}=0.22[o]
N_0V	0.407	0.407	-	-

a = [20];b = [11];c = [10];d = [62];e = [49];f = [12];g = [50]; h= [63]; i= [22];j= [54];k= [51];l= [53]; m= [15];n= [64];o= [47]; p= [65]; q=[66]; r=[18]; s=[24]; t=[19]; u=[48]; w=[1]; x=[67]; y = [17].

The present values of superconducting state parameters of MgB_2 for Model I and Model II along with relevant experimental data and other theoretical results are assembled in Table 3. It may be observed from Table 3 that the values of superconducting state parameters of MgB_2 obtained from the two approaches are in excellent agreement with each other. The T_c values calculated by us show excellent agreement with the experimental T_c value of 39K due to Nagamatsu et al. [1], and 39.25K obtained by Tomita et al. [67]. Also the experimental values of 39.2K due to Osborn et al.[20] and 38.7K due to Bonquet et al. [49] for $Mg^{11}B_2$ are in excellent agreement with the present values of T_c. The other theoretically reported values of T_c have been included in the last column of the Table 3. It may be seen that the values 39K by Choi et al. [15], 39.4K by Balaselvi et al. [47], 38.75K by Chen et al. [48] and 39.5 K by Neaton and Perali [64] show excellent agreement with the present results. The present T_c values are also well within the limit 37 to 42 K set by Choi et al. [15]

The present values of λ (=0.842) for MgB_2 also show good agreement with the value 0.9 reported by Osborn et al.[20] on the basis of inelastic neutron scattering measurements. The experimental value of λ reported by Kortus et al. [10] = 1.4 is on the higher side, whereas λ = 0.75 reported by An and Pickett [11], 0.58 by Wang et al. [62] and 0.62 by Bonquet et al. [49] on the basis of specific heat measurements are somewhat on lower side. Whereas most of the theoretical values of λ shown in the last column of Table 3 show good agreement with the present results, the value λ = 0.8408 obtained by Balaselvi et al.[47] is in the best agreement. Also the λ values, 0.907 and 0.922, reported for $Mg^{10}B_2$ and $Mg^{11}B_2$ respectively by Yildirim et al. [19] are in good agreement with the present results. The present λ values are also well within the limit 0.65 to 1.2 prescribed by Hinks et al. [18].

The same value of μ^* (= 0.124) is obtained for MgB_2 by us from the two approaches in the present formulation, which shows a good agreement with the value 0.12 reported by Choi et al. [15], 0.13 reported by Heid et al. [53], and lie well within the range 0.10 to 0.14 prescribed by Choi et al. [15], on the basis of anisotropic Eliashberg equations, including anharmonicity in the phonon frequencies.

The present formulation for the isotope effect exponent provides α= 0.462 for MgB_2 from both the models. This value is closer to the BCS value of 0.5 as compared to experimental values, α_B = 0.26 due to Bud'ko et al. [17] and α_B = 0.30 and α_{Mg} = 0.02 (i.e. α_{total}= 0.32) due to Hinks et al. [18]. Some of the theoretical results for α values of MgB_2 have been assembled in the last

column of Table 3. It may be observed that α_{total} = 0.36 and 0.50 predicted respectively by Choi et al. [15] and Osborn et al. [20] show better agreement with the present value of α (= 0.462). The fact that the present values of α from both the approaches are in excellent agreement with the value α_B = 0.46 obtained by Kong et al. [12] and the same also being quite close to the BCS value of 0.5, re-affirms that the origin of Superconductivity in MgB_2 may be attributed to the electron-phonon coupling.

In the absence of other values of interaction strength, an effective comparison of the present values of N_0V could not be possible, however the same value, N_0V = 0.407, obtained by us from both the approaches confirms the validity of the present formulation and reveals that MgB_2 is a strong coupling superconductor, in conformity with the observations of Kong et al. [12], Yildirim et al. [19], Kortus et al.[10], Kotegawa et al.[54] and Osborn et al. [20].

The presence of isotope effect in MgB_2 confirms the role of electron-phonon interaction i.e. electron-lattice interaction in the origin of superconductivity in this compound. In order to make this aspect more explicit, we investigate dependence of λ and T_c on the mass of Mg and B isotopes.

For this purpose we use two isotopes of Boron, i.e. ^{10}B and ^{11}B with masses 10.0051 and 10.9952 amu respectively [18] and three isotopes of Mg : ^{24}Mg, ^{25}Mg, and ^{26}Mg with their respective masses 23.985042, 24.985837 and 25.982593 amu [69]. In this analysis we also include three other isotopic masses of Mg used by Hinks et al. [18] for ^{24}Mg, ^{26}Mg and natural Magnesium, i.e., 24.001, 25.001 and 24.305 amu respectively. The dependence of T_c on isotopic mass of Mg and B for the two models has been shown in Fig.2. The slope of the linear graphs for T_c clearly depicts the dependence of T_c on isotopic mass of Mg and the separation between the T_c lines for ^{10}B and ^{11}B is a measure of the dependence of T_c on isotopic mass of B. Whereas the dependence of T_c on isotopic mass of B is quite prominent, the dependence of T_c on isotopic mass of Mg is also clearly visible from the slope of the T_c-graphs, which is now much better than that obtained by Hinks et al.[18]. We obtain for Boron isotopes δTc ~ 3.61K from the two models, as against δTc = 1K (Tc = 39.2K for Mg $^{11}B_2$ and 40.2K for Mg $^{10}B_2$) measured by Bud'ko et al.[17] and δT_c = 1.7K calculated by Kong et al. [12]. Hinks et al. [18] measured δT_c ~ 1.16K for Boron isotope effect in MgB_2, whereas Yildirim et al. [19] obtained δT_c = 0.8K, (T_c = 39.4K for Mg ^{10}B and 38.6K for Mg ^{11}B). Further, whereas the isotope effect

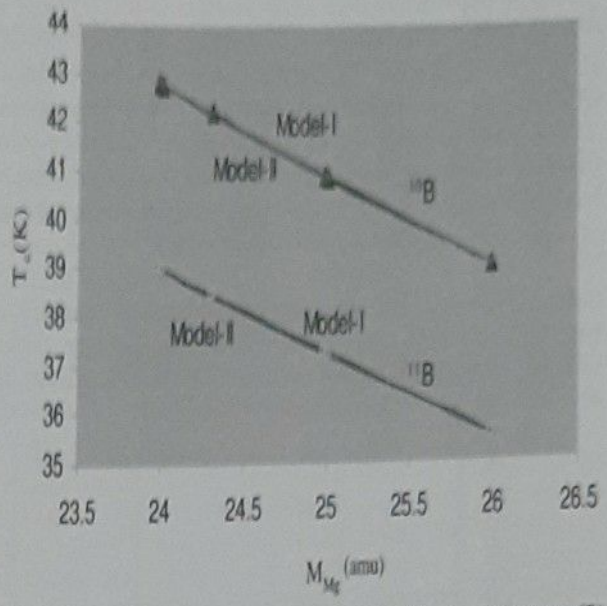

Figure 2. Variation of Superconducting transition temperature (T_c) with the isotopic mass of Mg for ^{10}B and ^{11}B isotopes of B, for the two models (Model-I & Model-II).

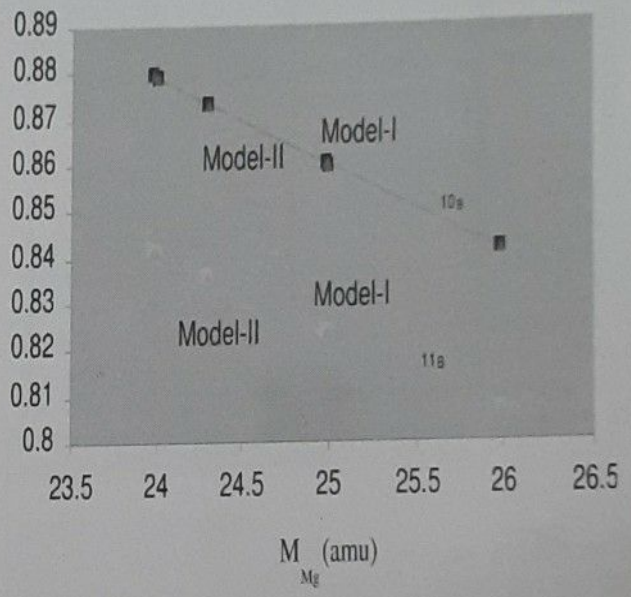

Figure 3. Variation of Electron-Phonon coupling strength (l) with the isotopic mass of Mg for ^{10}B and ^{11}B isotopes of B, for the two models (Model-I & Model-II).

of Mg isotopes on T_c was found to be negligibly small by Hinks et al. [18], in the present work we obtain δT_c ~ 3.64K from both the Models for mass variation of Mg isotopes.

The effect of the mass variation for B and Mg isotopes on λ in MgB_2 is also clearly visible from Fig. 3, in which we have plotted λ values obtained from the two models (model- I and II) against the isotopic mass of Mg. We obtain linear curves for the two isotopes of B

(^{10}B and ^{11}B). The slope of λ curves for each isotope of B clearly depicts the effect of Mg isotopes on λ, whereas the separation between the two λ-lines is due to the role played by B isotopes on the electron-phonon coupling in MgB_2. This proves the role of isotopic mass and the major role played by the boron planes in the superconductivity of MgB_2.

Further, in order to investigate electronic structure of Mg, B and MgB_2, we obtain Electron Energy Bands (EEB) and Density of States (DOS) for them by employing WIEN 2K10 code with Density Functional Theory in Generalized Gradient Approximation due to Perdew et al.[70]. The relevant diagrams of EEB and DOS for Mg, B and MgB_2 are shown in Figures 4, 5 and 6 respectively. It may be observed that whereas the valence band in B along ΓP direction and in MgB_2 along ΓA direction extend above the Fermi level and have vacant states, in Mg it lies well below the Fermi level with all the states filled up.

The presence of σ band along ΓA direction extending above the Fermi level and moderate DOS of the order of 0.71 states/eV in MgB_2 provide suitable conditions

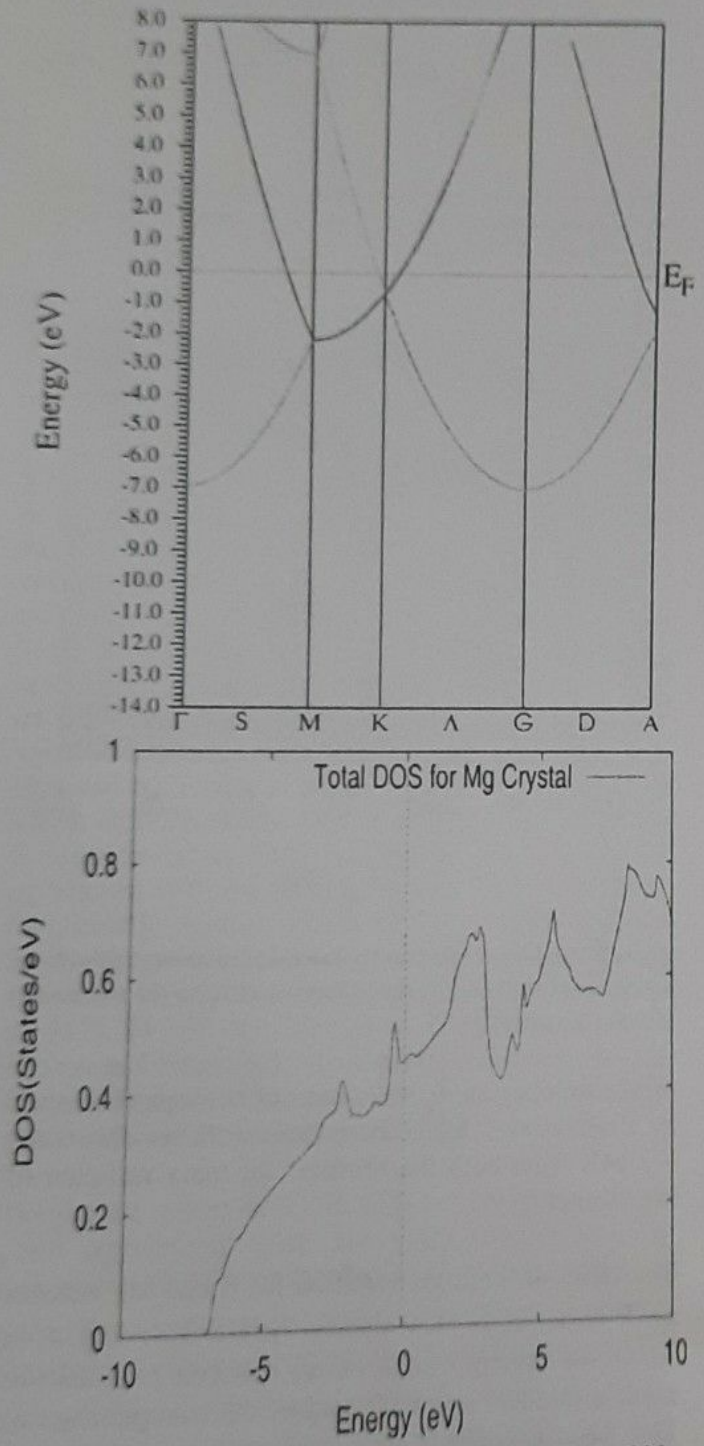

Figure 4. Electron Energy Bands and Density of States of Mg.

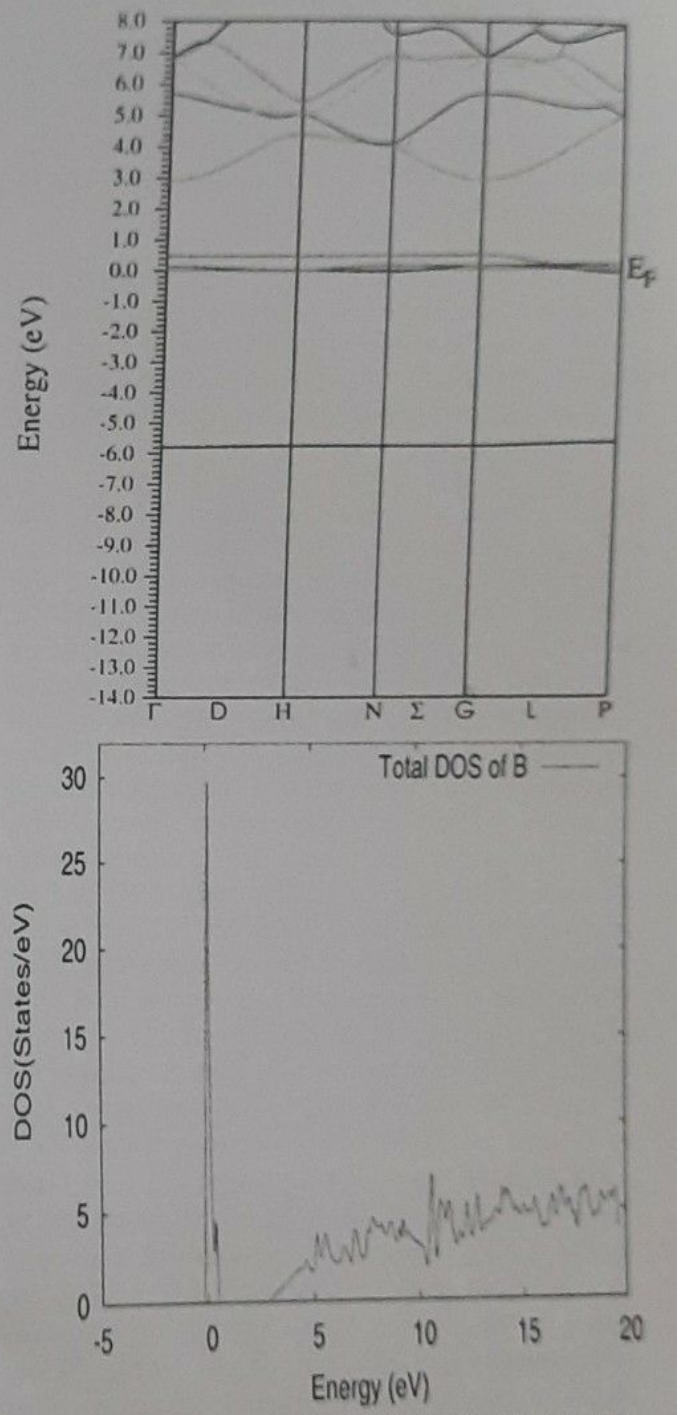

Figure 5. Electron Energy Bands and Density of States of B

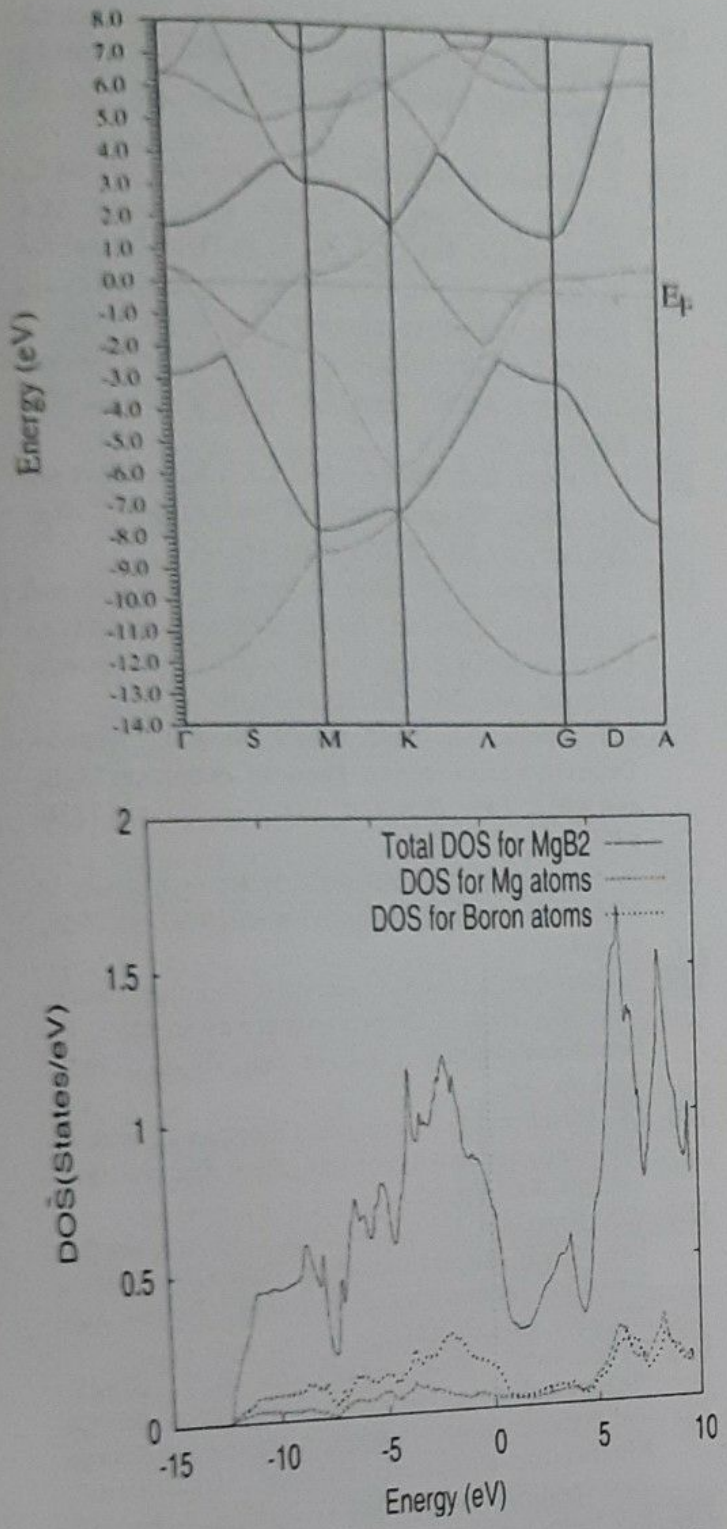

Figure 6. Electron Energy Bands and Density of States of MgB_2

for it to become superconductor at temperatures as high as 40K. In Mg the valence band along ΓA direction lies well below the Fermi level with all the states filled up and the DOS at Fermi level is also quite small, so that the conditions are not quite favourable for it to become a superconductor. This is in concurrence with the fact that it becomes superconducting at very low temperatures of the order of 0.017K. In the band structure of tetragonal Boron T-B_{50}, being reported for the first time, we obtain valence band along Γ P direction extending above the Fermi level with vacant states available for conduction to be possible. In the DOS of B, a sharp peak of height about 30 states/eV is observed at about the Fermi level, which makes conditions favourable for it to become a superconductor at moderate temperatures of the order of 11K on application of high pressure. The peak in the DOS of B, which disappears in the DOS of MgB_2, may play an important role in the observed superconductivity in MgB_2 at about 40K.

4 CONCLUSIONS

Present studies clearly establish that superconductivity in MgB_2 originates from electron-phonon interaction. The present investigations prove that BCS-Eliashberg-McMillan formulation, with pre-factor of T_c equation as suggested by Allen and Dynes, successfully explains superconductivity in MgB_2 in model pseudo potential approach. The present formulation successfully reproduces superconducting state parameters of Mg, B and MgB_2 in a unified manner. The role of isotopic mass is clearly established both for Mg and B isotopes, which proves that the electron-phonon interaction is the true cause of superconductivity in MgB_2.

The EEB and DOS obtained for MgB_2 suggest that the σ band along ΓA direction extending above the Fermi level and moderate DOS in it are responsible for a higher value of T_c in this compound. The high peak in the DOS of B at about the Fermi level, which disappears in MgB_2, may play an important role in the observed superconductivity in MgB_2. Further, whereas the EEB and DOS are favourable for B to become a superconductor on application of high pressure, the conditions are not so favourable for Mg.

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