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Calculation of superconducting transition temperature of MgB_2

M. Rajagopalan*, P. Selvamani, G. Vaitheeswaran, V. Kanchana, M. Sundareswari

Department of Physics, Anna University, Chennai 600 025, India

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Abstract

A theoretical calculation of the superconducting transition temperature is reported. The parameters that are necessary to calculate T_c are taken from the self-consistent band structure obtained by means of the TB-LMTO method. The calculated value of T_c is in good agreement with the experimental value. From the present calculation, we observe that the high T_c may be due to the metallic nature of boron sheets and the phonon mediated mechanism can be employed to explain T_c in these compounds.

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The recent discovery of superconductivity in magnesium diboride (MgB_2) with T_c as 39 K caused excitement in the Solid State Physics community [1]. MgB_2 is a new simple intermetallic superconductor with a high superconducting transition temperature for a nonoxide and a non C_{60} based compound. The reported value of T_c seems to be either above or at the limit suggested theoretically for BCS, phonon mediated superconductivity [2]. In this paper, we report a theoretical calculation T_c using McMillan's formula [2]. The inputs that are used to calculate T_c are taken from the self-consistent band structure calculation by Tight Binding Linear Muffin-Tin Orbital method (TB-LMTO).

MgB_2 crystallizes in the hexagonal AlB_2 type structure (space group no. 191), which consists of alternating hexagonal layers of Mg atoms and graphite like layers of B atoms. The lattice parameters ($a = 3.0834$ Å and $c = 3.5213$ Å) are taken from the experimental work [3]. The atomic positions are Mg at (000) and B at (1/3,2/3,1/2). The electronic structure is obtained by TB-LMTO method within the atomic sphere approximation. The exchange correlation potential with the local density approximation is calculated using the parameterization scheme. The sphere radii are chosen in such a way that there is a charge flow from Mg to B as per electro negativity criteria. The band structure calculations are performed for 10,648 K points within the entire Brillouin Zone. The convergence for K and E are checked by increasing the number of K points. The total and projected density of states at Fermi level is obtained by tetrahedron method. The total density of states at the Fermi level is 8.693 states/Ryd/F.U. Using this value, the electronic specific heat coefficient is calculated using the expression

$$\gamma = 2/3\pi k_B^2 N(E_F) \tag{1}$$

which comes to around 1.5 mJ/mol-K^2. Recently Bud'Ko et al. [4] measured the specific heat coefficient and reported a value of 3 ± 1 mJ/mol-K^2. From the experimental and theoretical value of γ, one can estimate the electron–phonon coupling constant, λ, using the expression

$$\gamma_{exp} = \gamma_{the}(1 + \lambda). \tag{2}$$

Using this expression the value of λ is found to be 1.0 which gives an indication that superconductivity in MgB_2 may be due to phonon-mediated mechanism.

The superconducting transition temperature is calculated using McMillan's formula.

$$T_c = \frac{\Theta_D}{1.45} \exp\left\{\frac{-1.04(1 + \lambda)}{\lambda - \mu^*(1 + 0.62\lambda)}\right. \tag{3}$$

where Θ_D is the Debye temperature and μ^* is the electron–electron interaction parameter. The electron–phonon coupling constant for MgB_2 is calculated using Phillip's

* Corresponding author. Tel.: +91-44-2403023; fax: +91-44-2352870.

E-mail address: mraja@eth.net (M. Rajagopalan).

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formula [5] which is

$$\lambda = \lambda_A + \lambda_B \tag{4}$$

$$\lambda = \frac{N_A(E_F)\langle I_A^2\rangle}{M_A\langle\omega_A^2\rangle} + \frac{N_B(E_F)\langle I_B^2\rangle}{M_B\langle\omega_B^2\rangle} \tag{5}$$

where A and B stand for the metal and non-metal atoms in the compound. The quantities $N_A(E_F)$ and $N_B(E_F)$ which are the densities of states at Fermi energy for the A and B atoms in the compound are obtained from the band structure calculations. This kind of separation is valid when the difference in the masses is large ($M_A > M_B$).

$\langle I^2\rangle$ is the square of the electron–phonon matrix element averaged over the Fermi surface. The parameters necessary to calculate the matrix element are taken from the self-consistent band structure results and $\langle I^2\rangle$ are calculated both for Mg and B atom sites in a manner similar to our earlier work [6].

The value of the Debye temperature for the compound is taken as 750 K [4]. However, to calculate the values of λ_A and λ_B one needs information about the partial character of the phonon spectrum which is not available. Since the difference in masses is large, the following approximation is used to calculate $\langle\omega_A^2\rangle$ and $\langle\omega_B^2\rangle$.

By virtue of mass inequality, the metallic atoms oscillates in the acoustic frequency range and the non-metal in the optical frequency range. This approximation can be written as

$$\langle\omega_A^2\rangle \approx 1/M_A \qquad \langle\omega_B^2\rangle \approx 1/M_B \tag{6}$$

$$\langle\omega_A^2\rangle/\langle\omega_B^2\rangle \approx M_B/M_A \tag{7}$$

The value of Θ_D for Mg is taken from the literature and that of B is calculated using the above expression by setting $\langle\omega^2\rangle = 0.5\Theta_D^2$. The calculated values of $\langle\omega_A^2\rangle$and $\langle\omega_B^2\rangle$ are used to compute λ_A, λ_B and λ for the compound. The value of λ is found to be 1.04 which is in good agreement with the earlier work ($\lambda = 0.9$) [7]. With this λ value, T_c is calculated by using McMillan's formula and found to be 39.53 K., in agreement with the experimental value. The B isotope shift of T_c reported Bud'ko et al. [4] and most other experimental data suggest conventional BCS strong coupling s-wave electron–phonon pairing in MgB_2. So in the present work, McMillan formula which is based on the BCS theory is used. The value of μ^* is taken as 0.1

Taking the logarithmic volume derivative of T_c and obtain the simple relation,

$$\frac{\mathrm{d}\ln T_c}{\mathrm{d}\ln V} = -\nu + \left\{\Delta\frac{\mathrm{d}\ln\eta}{\mathrm{d}\ln V} + 2\nu\right\} \tag{8}$$

where $\nu = -\mathrm{d}\ln\langle\omega\rangle/\mathrm{d}\ln V$ is the Grunesian parameter, $\eta = N(E_F)\langle I^2\rangle$ is the Hopfield parameter given by the product of the electron density of states and the average of the square of the phonon matrix element and Δ can be written as [7]

$$\Delta = \frac{1.04\lambda[1 + 0.38\mu^*]}{[\lambda - \mu^*(1 + 0.62\lambda)]^2} \tag{9}$$

Using the above relation Δ value obtained in the present case is found to be 1.67 which is in good agreement with the earlier work $\Delta = 1.75$ [7].

Table 1

MgB_2	Partial density of states			λ	T_c (K)
	s	p	d		
Mg	0.34	0.60	0.87	0.39	39.53
B	0.18	5.76	1.01	0.65	

The parameters that are entering into the calculation of T_c are given in Table 1. Moreover, it was pointed out [8–11] that super conductivity in MgB_2 is essentially due to metallic nature of Boron sheets. From this work we observe (Ref. Table 1) that the contribution to the total density of states mainly comes from boron atoms which supports the view point that superconductivity is essentially due to metallic nature of boron sheets.

In summary, the superconducting transition temperature of MgB_2 has been calculated using the output from self-consistent band structure calculations by employing McMillan's formula. The theoretically calculated value of T_c (39.53 K) is in very good agreement with the experimental observation. From the band structure results, we observe that the contribution to the density of states is mainly from the boron atom. This suggests that superconductivity may be due to the metallic nature of boron sheets and the value of λ suggests that superconductivity may be due to a phonon-mediated mechanism.

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