Theoretical Investigation on Occurrence of Unconventional Superconductivity in $Mg_{(1-x)}T_xB_2$ Compounds

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Abstract

The structural, bonding, magnetic, electronic, elastic and thermoelectric nature of superconducting material namely MgB_2, with hexagonal structure (space group is 191) are studied by first principle calculation. The optimized lattice parameters of MgB_2 are a=b=3.084289 Å and c= 3.51527 Å and the electron phonon coupling constant (λ), Debye temperature, critical temperature, Seebeck coefficient, electrical resistivity and the elastic constants (C_{11}, C_{12}, C_{13}, C_{33}, C_{55}) are calculated and agreed well with available outcome. To predict other possible superconducting materials belong to MgB_2 family, Mg is further doped with transition element Titanium (Ti) and analyzed. Copyright © VBRI Press.

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Introduction

As a superconducting material MgB_2 plays a major role in recent years due to its critical temperature, T_c = 40K for binary compound. It has special features like, trouble-free structure and high transition (T_c) temperature [**1**]. Since the bonding between B-B is strong covalent results good electron phonon coupling factor which is liable for high value of transition (critical) temperature in MgB_2 compound [**2, 3**]. To prove the validity of our studies, initially a complete band structure calculation for MgB_2 and to propose a new possible superconducting material has executed. Here we have chosen the transition element Titanium (Ti) as a dopant due to its high conductivity. By doping Ti with Mg, it enhances the superconducting properties under temperature [**4**]. In this paper we have reported the optimized parameters of the hexagonal structured MgB_2 and $Mg_{0.5}Ti_{0.5}B_2$ with the space group 191(P6/mmm). The structural factors of $Mg_{0.5}Ti_{0.5}B_2$ compound initially predicted from MgB_2 and the position parameters for Mg, B, and Ti are (0, 0, 0), (1/3, 2/3, 1/2) and (0, 0, 1/2) respectively.

Computational method

The methodology is executed by Full Potential Linearized Augmented Plane Wave scheme as employed in WIEN2K software code [**5**]. The Generalized Gradient - Approximation (GGA) parameter scheme has used to find exchange correlation potential [**6**]. Radius of Muffin tin spheres (RMT) is preferred due to its minimal leakage of charge from the core. The spin and non-spin polarization is performed with optimal K-points with minimum convergence for charge, forces and energy. The total energy is calculated by volume and pressure relation executed by Birch and Murnaghan equation of state [**7**].

The complete structural factors of the experimentally reported MgB_2 compound are optimized and compared. The calculated (electronic) specific heat parameter (γ) and Debye temperature are applied in a Mc'Millians formula, the transition temperature (T_c) was calculated for the MgB_2 compound. The a Mc'Millians formula is expressed as $T_c = (\Theta_D/1.45) \exp [- (1.04) (1+\lambda) / (\lambda-\mu^*-0.62\mu^*\lambda)]$ where, Θ_D - Debye's factor for temperature and μ^* electron- electron interaction ($\mu^* = 0.1$) [**8**]. The lattice parameters and the positional parameters of $Mg_{0.5}T_{0.5}B_2$ are optimized by volume optimization, c/a optimization and position minimization.

Result and discussion

(a) Structural, electronic and magnetic properties of MgB_2 and $Mg_{0.5}Ti_{0.5}B_2$ Compounds

The first part of work is the optimized band structure calculation of MgB_2 compound to explore the physical, magnetic and electron transport property of the compound. The obtained results are tabulated in **Table 1**. To analyze the magnetism behavior, the spin-orbit coupling execution has been carried out. The diamagnetism behavior of the compound has revealed by the observed least magnetic moment value. The theoretical calculation of (electronic) specific heat coefficient (γ_{th}) is calculated by using the relation, $\gamma_{th} = (\pi^2/3)K_B^2N(E_F)$. Where, K_B is the Boltzmann constant. The (electron–phonon) coupling (λ) constant value is obtained by, $\lambda = (\gamma_{expt}/\gamma_{th})-1$ [**9**]. Then Density of States histograms and plot of band structures are

analyzed to explore the electron transport behavior over conducting nature of material shown in **Fig. 1** and **Fig. 2**. The band structure of MgB_2 and $Mg_{0.5}T_{0.5}B_2$ shows the motion of the electrons over the Fermi energy level, proves the conductivity and it gives that the conductivity range is higher in titanium doped MgB_2. The DOS in MgB_2 depicts more contribution arises from Boron; and in $Mg_{0.5}Ti_{0.5}B_2$ more contribution arises from Ti. **Fig. 1(c)** and **Fig. 2 (c)** shows Fermi surface of MgB_2 and $Mg_{0.5}Ti_{0.5}B_2$ respectively and it shows the electron cylinders at A point and sheets over K points implies it conducting phenomenon.

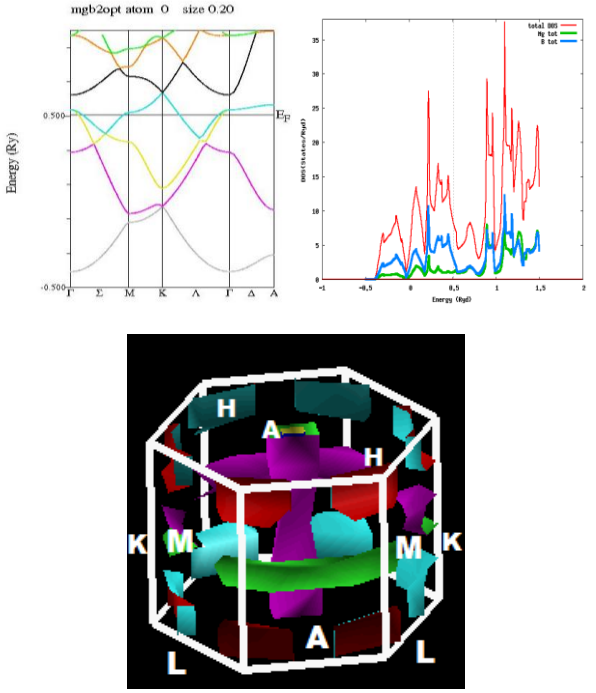

Fig. 1. MgB_2 (a) Band structure profile (b) DoS histogram (c) Fermi surface.

(b) Bonding and Mechanical properties of MgB_2 and $Mg_{0.5}Ti_{0.5}B_2$ Compounds

Density plots of electron (**Fig. 3**) and the inter atomic distances are examined to know the bonding between the atoms in a compound, which is expressed as (Mg, Mg) is 5.2885 a.u, (B, B) is 3.3651 a.u, and (Mg, B) is 4.7282 a.u for MgB_2 and (Mg, Mg) is 6.9912 a.u, (Mg, Ti) is 51793 a.u and (Ti, B) is 4.034 a.u for $Mg_{0.5}$ $Ti_{0.5}B_2$. The **Fig. 3a** depicts the bonding between Mg and B is ionic and agreed with the literature. **Fig. 3b** shows that covalence is exists in between Boron atoms by distributing uniform contours that around B-B atoms; Ionic bonding is exist in between B and Mg (Ti).

The universal anisotropic factor is expressed as, $A^U = 5\ G_v / G_R + (B_v / B_K) - 6$. If A=0, then there is no anisotropic in the compound. If $A \neq 0$, then the compound is a high anisotropic nature. The elastic modulus values; Poisson's ratio (σ), Young's (E), Shear (G) and Bulk (B) are offered in **Table 1**. By our study the compound MgB_2 and $MgTiB_2$ exhibit a high anisotropic nature. To be aware of the brittle (or) ductile nature, the Pugh's criterion (G/B) is provided. If G/B is more than (>) 0.57, represents brittle nature or it represents ductile nature [**15**]. Here the G/B (ratio) for MgB_2 is 0.5152, is ductile in nature and for $Mg_{0.5}Ti_{0.5}B_2$ the G/B ratio is 2.6014, is brittle in nature therefore by doping a compound it changes its mechanical property.

Table 1. The optimized structural, magnetic, electronic and elastic parameters of MgB_2 and $Mg_{0.5}Ti_{0.5}B_2$ compounds.

Parameters	**MgB_2**	**$Mg_{0.5}Ti_{0.5}B_2$**
Lattice parameter (a) Bohr	3.0843(3.0834[10]; 3.087[11])	3.6996
Lattice parameter(c) Bohr	3.5153 (3. 5213[10] ;3.524[11])	5.48155
Fermi energy (E_F) Ryd.	0.5068	0.44238
DOS [$N(E_F)$] Ryd.	8.42 (8.93[10]; 9.98[11])	8.10324
(Electronic) Specific (γ) heat (mJ/(mol cell K**2)	1.46 (1.6[10] ; 3.06[11])	1.4038
Electron phonon coupling λ	1.10 (1.04[10] ; 1.84[11])	0.6767 (approx.)
Critical temperature (T_c)	55.0303 K (39.53 K[10]; 38.6 K[11])	31.57 K
Debye temperature, θ_D	863.65 K (750 K[10])	1193.97 K
C11 (GPa)	321.276 (524[12]; 433.85[13])	351.0252
C12 (GPa)	157.786 (58[12]; 68.86[13])	-15.7509
C13 (GPa)	50.459 (33[13]; 44.61[14])	-8.0458
C33 (GPa)	225.444 (243[12]; 265.30[13]	179.4437
C55 (GPa)	55.852 (85 [12]; 74.06 [13])	347.0476
Bulkmodulus (GPa) $B_{voigt}/B_{REUSS}/B_{HILL}$	153.94/141.330/147.629	90.67/82.651/ 886.759
Shear modulus (GPa) $G_{VOI}/G_{REUSS}/G_{HILL}$	79.311/72.202/72.756	236.385/194.171/ 215.278
Young's modulus (GPa) $Y_{VOI}/Y_{REUSS}/Y_{HIL}$	203.051/185.087/194.071	379.806/326.686/ 353.472
Poisson's coefficient, $P_{VOI}/P_{REUS}/P_{HIL}$	0.250/0.281/0.280	-0.196/-0.158/ -0.179
Magnetic moment, μ_B	0.00036	-0.7223
Pugh Ratio (G/B)	0.5152	2.6014
A^U	0.5349	0.1892

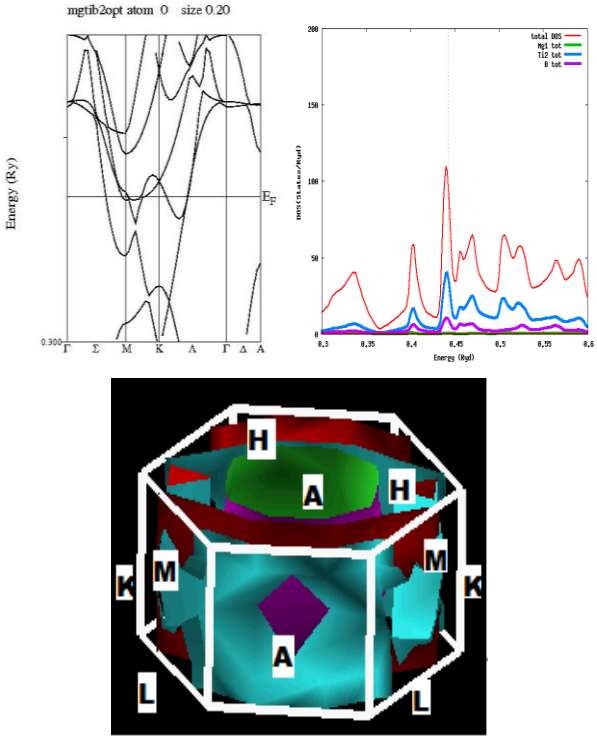

Fig. 2. $Mg_{0.5}Ti_{0.5}B_2$ (a) Band structure profile (b) DoS histogram (c) Fermi surface.

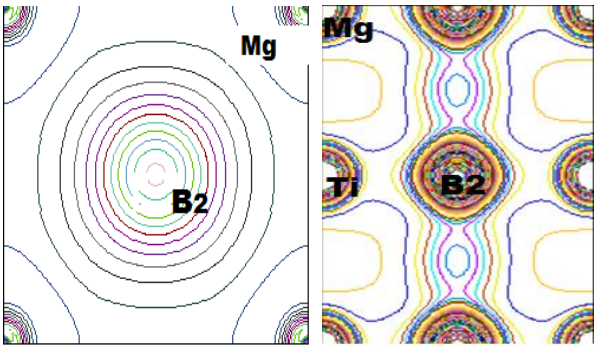

Fig. 3. Electron density plot a) MgB_2 b) $Mg_{0.5}Ti_{0.5}B_2$.

(c) Thermoelectric properties of MgB_2 and $Mg_{0.5}Ti_{0.5}B_2$ compounds

Table 2. Thermoelectric parameters of MgB_2 and $Mg_{0.5}Ti_{0.5}B_2$ compounds.

	Conductivity (σ) $\Omega^{-1}m^1$		Resistivity, ρ μΩ cm		Seebeck coefficient	
	MgB_2	**$Mg_{0.5}Ti_{0.5}B_2$**	**MgB_2**	**$Mg_{0.5}Ti_{0.5}B_2$**	**MgB_2**	**$Mg_{0.5}Ti_{0.5}B_2$**
100	2.2919	6.0112	4.363	0.1663	1.619	0.26222
200	1.6758	2.5633	5.967	3.90124	4.525	0.26206
300	1.2100	1.0022	8.2640 $(8.7)^4$	0.9978	6.915	0.25771 2
400	5.8016	3.735	1.7236	0.2677	8.5179	0..25619
500	3.4224	8.2188	2.9219	0.1267	9.4810	0.2573
600	4.0183	1.0684	2.4888	0.9359	1.0031	0.2604
700	6.2928	1.00364	1.5890	0.9637	1.0350	0.2646

BoltzTraP code is used to analyze the thermoelectric properties [**16**]. The given table explains the change in conductivity and resistivity with respect to temperature in its corresponding Fermi energy states. At 300 K the conductivity nature of both materials under study is same, hence in forth this study used to predict novel superconducting materials and the same proved by theoretical values. At below the room temperature $Mg_{0.5}Ti_{0.5}B_2$ exhibits more conductivity than MgB_2. Here, in novel material namely $Mg_{0.5}Ti_{0.5}B_2$, 'S' is very less and 'σ' is high than parent compound namely MgB_2.

Conclusion

The structural, magnetic, elastic and electronic properties of a doped material $Mg_{0.5}Ti_{0.5}B_2$ are predicted. Pugh's ratio shows that the mechanical property of MgB_2 inverted into brittle by doping Ti with Mg in 50%. Both the compounds have high anisotropy bonding nature and the same is proved by using the universal anisotropy index (A^U). The conductivity nature of both the compounds is similar at room temperature and $Mg_{0.5}Ti_{0.5}B_2$ reveals more conductivity at low temperature. The more contribution towards DOS arises from Boron in MgB_2 and from Titanium in $Mg_{0.5}Ti_{0.5}B_2$. In both the compounds the covalence is exist in between the boron atoms and ionic nature is exist in between Boron with other atoms.

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