Advances in Physics Theories and Applications
ISSN 2224-719X (Paper) ISSN 2225-0638 (Online)
Vol.83, 2020

The Study on Effect of Carbon© on the Electronic Structure of $MgB_XC(x = 1, 2)$

M. A. Afrassa
Adama Science and Technology University, Adama, Ethiopia

Abstract
In this work first principle study on electronic structure calculations for MgBC, and MgB_2C is presented. The density functional theory (DFT) as implemented in Quantum-ESPRESSO was used. The band structure and density of state (DOS) is compared with the already reported MgB_2. It is clearly observed that the presence of Carbon in both compounds change the Fermi level and the hole bands. In MgB_2C the Fermi level is higher than MgBC that results in suppression of Tc in MgB_2C. In MgBC the hole band shifted up from gamma to X direction and this may improve superconductivity of the material. Comparison of the DOS at the Fermi level reveals that MgBC has the highest value (0.9424 state/cell/ev). Using reasonable approximations, the calculated Tc values are, 27.07k and 41.09k for MgB2C and MgBC respectively. This suggests that Carbon(C) has a better contribution than Boron(B) and MgBC is a good candidate for high Tc.
Keywords: Superconductivity, Band structure, Density of state(DOS), Density Functional theory(DFT)
DOI: 10.7176/APTA/83-03
Publication date: February 29th 2020

1. Introduction

Superconductivity has been observed in different class of materials including organic superconductors, A 15 compounds, heavy fermions, Cupraites, chalcogens, and Iron based superconductors. These classes of materials are not yet well understood and so far there is no report that indicates superconductivity at room temperature. Different experimental and theoretical methods have been employed in order to understand the onset of superconductivity and to increase superconducting critical temperature Tc to room temperature.

In 2001 MgB2 was found to be superconducting with the critical temperature of 39K [1]. This compound, MgB2, is a metallic material and the superconducting properties have been reported [2-6]. It is an attractive candidate for practical applications [7]. Different report indicated that the superconducting mechanism in MgB2 is phonon-mediated [8, 9]. Different attempts were reported to study the superconductivity of MgB_2 and to improve Tc by substituting different elements including Aluminum (Al) and Carbon(C). Superconductivity was reported by doping different element but Tc was not significantly increased [10, 11].

Aluminum (Al) doping on Magnesium (Mg) site showed that Tc is suppressed [12] and superconducting gap is reduced [13]. Al substitution is an electron doping that reduce hole bands, and this may be the reason for suppression of Tc. The other report was Lithium (Li) doped MgB_2[14]. In this case Tc is reduced but the effect is less compared to Al doped MgB_2. On the other hand the effect of Carbon© doping on Boron (B) site also reported and shows different properties [15, 4,5,7]. Theoretical report indicated that MgB_2C_2 is a good candidate for high superconductivity [16].

It is common to read articles on the electronic structure calculation computationally that provides a significant result in understanding the superconductivity of many compounds. In this computational work we attempt to understand the effect of carbon on the electronic structure of magnesium diboride related compounds. We particularly compared the electronic band structure and DOS of MgB_2, MgB_2C, and MgBC.

2. Computational details

In this work first principle calculation in Density Functional Theory (DFT) as implemented in Quantum ESPRESSO (QE) [17] was applied to calculate the electronic band structure, Crystal structure and density of state for MgB_2, MgBC, and MgB_2C. The experimental value of the lattice parameter (a and c) from literature is used. The bands are plotted along the high symmetry direction Γ-M-K-Γ-A-L-H-A|L-M|K-H in the Brillouin zone of Hexagonal lattice [18]. The DOS calculations were performed using tetrahedron method. In general it is nonmagnetic calculations.

3. Result and discussion

(a) Electronic Band structure calculation

It is reproduced the known band structure of MgB_2 in order to compare and see the effect of Cobalt (Co) substitution. The band structures are plotted along the high symmetry of Gamma-M-k_A-L-H-A direction of the Brillouin zone. The effect of Co substitution on the number, shape and size of bands are checked. In all calculations it is found that there are bands that cross the Fermi level, indicating the multi band nature of the compounds. The results are shown in the Fig 1, and Fig 2.

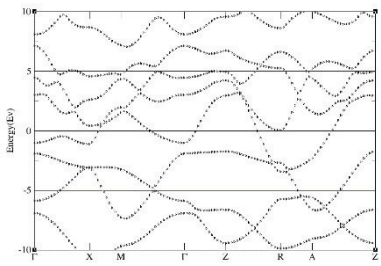

Figure 1: Band structure of MgBC

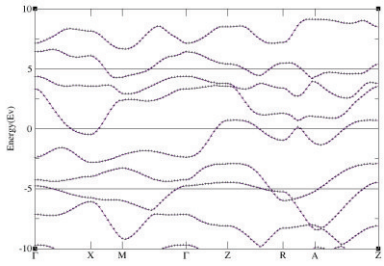

Figure 2: Band structure of MgB2C

In the band structure of MgB_2C, Figure 1, we can observe that unlike for MgB_2 From gama to M, there are one electron and one hole in between 0eV to 2.5eV. Also, there is a flat band above a Fermi level in between 5 ev to 10 ev from gama to Z. There is a curvature above and below the Fermi surface. From M – A. In this system due to the flatness of the bands, there are only a few numbers of bands cross the Fermi level.

The electronic band structure of MgBC (carbon substitution in place of one Boron) is as shown on the figure 2. There is a band break from X-M, due to the absence of one Boron and replaced by one carbon. This character is around the Fermi energy of -10 ev. There is the appearance of band gap and flat band properties from gamma-Z in between the Fermi energies of 5ev and 10ev. There is also band dispersion (overlap) above a Fermi level in between 0ev and 5ev, from gamma-Z and also a band curvature in similar band widths, in between the Fermi energy of -10ev and 0ev. When we compare it with the structure on the other two there are quite bands crossing the Fermi level.

In general, in the presence of two boron in MgB_2C, the bands are moved up and so the Fermi level has a higher energy compare to MgBC. This may be the reason for the suppression of Tc in MgB_2C. On the other hand, substitution of Carbon in presence of one boron(MgBC), shift up the hole band from gama to x direction and this may improve the superconductivity of the material.

(b) Density of electronic state

Figure3-4 shows the calculated density of state for MgBc and MgB_2C respectively. The zero point is the Fermi level. The behavior of both graphs is similar with MgB_2 except that the DOS value at the Fermi level is different. For comparison purpose we calculated DOS of MgB_2 even though MgB_2 was already reported.

Table 1: The calculated DOS and Tc of MgBC, MgB_2C and MgB_2

	MgBC	MgB2C	MgB2
Density of state(DOS)	0.9424 state/cell/ev	0.6897state/cell/ev	0.7540 state/cell/ev
Tc	41.09k	27.07k	37.34

Using the theoretical value of DOS in the well-known McMillan equation and reasonable approximations I calculated the critical temperature Tc as shown in the table 1.

The DOS and TC of MgBC is high compare to the other. This approximation suggested that MgBC is a better candidate for higher Tc and further experimental work.

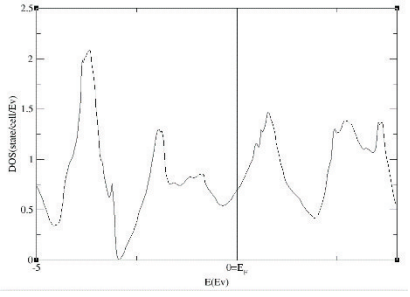

Figure 3: DOS of MgB2C

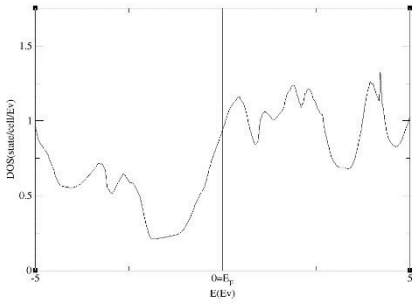

Figure 4: DOS of MgBC

4. Summary

In summary, the study focused on the effect of Cobalt(Co) substitution using Density Functional theory(DFT) as implemented in Quantum espresso. The effect is clearly seen on the band structure and DOS of MgBC and $MgBC_2$ with respect to MgB_2. MgBC is characterized by highest density of state and critical temperature compared to MgB^2 and MgB2C. From this we conclude that, after carbon is added to the super conducting MgB_2 in place of one Boron, the band structure, the density of state and the critical temperature are all changed. and the most important finding of the researcher was that, carbon has a great contribution than boron in case of increasing critical

temperature and density of state and MgBC can be another compound having high critical temperature.

REFERENCE

[1]. D.Dew-Hughes,Lowtemp. Physics**.27** ,99-102(2001).
[2]. B.K.Godwal et al;current.science.vol**85 ,**NO 7,10,(2003) .
[3] Jun Nagamatsu et al,Nature,Vol**,410,**(2001)
[4] Y. W. Maz,l. Phys. Lett. ,vol**. 88,** p. 505(2009)
[5] W.K.Yeohetal supper. SciTeechl V **19,**196- 5949(2006).
[6] Sergy L. et al; arXiv;.150106948 v**1** [cond-mat.suppr-con] 27 Jan 2015
[7] Y. Zhao, s" Appl. Phys.Lett.Vol**.83**, p.2916 (2003).
[8] H. L. Xu,"Chin.Phys.Lett.**Vol.21** ,25 -113**,(**2004).
[9] Karol Szałowski, Phys.Rev. B 74, 094501 (2006)
[10] A. P. Tiwari, et. al, Journal of Physics: Condensed Matter 29, 445701 (2017).
[11] S. Nishiyama, et al., Scientific Reports 7, 7436 (2017)
[12] T. Dahmand N. Schopohl, Phys. **Rev. Lett. 91** (2003) 01700
[13] E. C. Park, et.al, IEEE Transactions on Applied Superconductivity,19, 3 (2009)
[14] J. Karpiski, et,al, Physica C 456, 3 (2007).
[15] J. H. Kim nanotubes,et al" Appl. Phys. Lettv**89 ,** 122510 (2006)**.**
[16] P. Ravindran, et, al. Phys.Rev.B 64, 224509 (2001).)
[17] P. Giannozzi et al., J.Phys.:Condens. Matter 21 395502 (2009);
[18] Wahyu Setyawan and Stefano Curtaro, Computational Materials Science 49 (2010) 299–312