The Study on Effect of Carbon© on the Electronic Structure of MgBxC(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\textsubscript{2}C 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\textsubscript{2}. It is clearly observed that the presence of Carbon in both compounds change the Fermi level and the hole bands. In MgB\textsubscript{2}C the Fermi level is higher than MgBC that results in suppression of Tc in MgB\textsubscript{2}C. 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 MgB\textsubscript{2}C 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 MgB\textsubscript{2} was found to be superconducting with the critical temperature of 39K [1]. This compound, MgB\textsubscript{2}, 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 MgB\textsubscript{2} is phonon-mediated [8, 9]. Different attempts were reported to study the superconductivity of MgB\textsubscript{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\textsubscript{2}[14]. In this case Tc is reduced but the effect is less compared to Al doped MgB\textsubscript{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\textsubscript{2}C\textsubscript{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\textsubscript{2}, MgB\textsubscript{2}C, 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\textsubscript{2}, MgBC, and MgB\textsubscript{2}C. 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\textsubscript{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\textsubscript{L}-M|K-H in 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.
In the band structure of MgB$_2$C, Figure 1, we can observe that unlike for MgB$_2$ from gamma to M, there are one electron and one hole in between 0 eV to 2.5 eV. Also, there is a flat band above a Fermi level in between 5 eV to 10 eV from gamma 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 5 eV and 10 eV. There is also band dispersion (overlap) above a Fermi level in between 0 eV and 5 eV from gamma-Z and also a band curvature in similar band widths, in between the Fermi energy of -10 eV and 0 eV. 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$_2$C, 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 $T_c$ in MgB$_2$C. On the other hand, substitution of Carbon in presence of one boron (MgBC), shift up the hole band from gamma to x direction and this may improve the superconductivity of the material.

(b) Density of electronic state

Figure 3-4 shows the calculated density of state for MgB$_2$C and MgBC 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 $T_c$ of MgBC, MgB$_2$C and MgB$_2$

|        | MgBC     | MgB$_2$C | MgB$_2$ |
|--------|----------|----------|---------|
| Density of state (DOS) | 0.9424 state/cell/ev | 0.6897 state/cell/ev | 0.7540 state/cell/ev |
| $T_c$  | 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 $T_c$ 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 $T_c$ and further experimental work.

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 MgB$_2$C. From this we conclude that, after carbon is added to the superconducting 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. vol85, NO 7,10,(2003).
[3] Jun Nagamatsu et al, Nature, Vol. 410, (2001)
[4] Y. W. Mazl. Phys. Lett., vol. 88, p. 505 (2009)
[5] W.K. Yeoh et al; supper. SciTeechl V 19, 196- 5949 (2006).
[6] Sergy L. et al; arXiv:150106948 v1 [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