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UNDERSTANDING THE ELECTRONIC PROPERTIES OF BORON DOPED SILICON CARBIDE

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ABSTRACT
Semiconductor materials, with qualities such as fast speed, ease of processing, and a wide temperature range, constitute the foundation of modern electronics. The best feature is that they can be doped with impurities to change their characteristics in a controlled fashion. SiC, a wide bandgap semiconductor offers electrical features that make it ideal for high-power and high-frequency applications. In order to use SiC in electronics devices, it's critical to understand its properties. Different characteristics such as the lattice constant, band gap, band plot, and density of states are determined in this work using the first principle of Density Functional Theory. The band structure was calculated, displayed, and the band gap was determined. The band energies of SiC doped with Boron were computed. The densities of states as well as the band structure with the impurity were plotted. To determine the effect of Boron doping on SiC, the findings obtained before and after doping were compared.

Key words: Semiconductor, Modern Electronics, SiC, Density Functional Theory

1. INTRODUCTION
In the electronics sector, semiconductor materials have played a critical role. They are especially essential since their conductivity can easily be affected by changing conditions like as temperature and impurity concentration. The electrical conductivity and band gap of semiconductors are used to classify them. A semiconductor acts as an insulator at very low temperatures but has strong conductivity at ordinary temperatures. Semiconductors have a band gap of less than 3 eV, while insulators have a band gap greater than 3 eV. The boundary, however, is not particularly sharp. Wide bandgap semiconductors include SiC (band gap:2.3 to 3.4 eV), GaN (3.4 eV), diamond (5.5 eV), ZnS (3.6 eV), and others with band gaps approaching or above the upper limit.

Since its inception, silicon has dominated the electronics industry. However, with the development of high-speed microprocessors, smaller transistor sizes, and rising need for higher-efficiency electronics in severe environments, silicon's limitations are becoming more apparent. Silicon-based transistors have a temperature limit of a few GHz and are extremely sensitive to severe conditions. Wide bandgap semiconductors (e.g. SiC, GaN, and ZnO) on the other hand, are superior to silicon in terms of physical (e.g. high melting point, hardness, and so on) and electrical properties. Silicon Carbide (SiC) is a broad bandgap semiconductor with unique electrical properties that make it ideal for high power and high frequency applications.It has high breakdown electric field (1 to 2.5×10^8 V/m for different polytypes), high thermal conductivity (4.9Wcm-1k-1) and high inertness.

The tetrahedral structured SiC crystalizes in different polytypes (Davis, 1993). Properties such as the breakdown electric field strength, which allows the material to withstand up to certain voltage, is quite high for SiC in comparison to Si because of the wide band gap. The use of SiC, can enable the high power devices to operate in higher value of blocking voltage. High thermal conductivity, and high emissivity in the infrared also makes SiC a preferable choice for high temperature uses. Its high thermal conductivity enables more efficient removal of heat from the device. The high electrical resistance of SiC has been used to advantage in resistive heating applications such as igniters for natural gas furnaces. On the whole, one can say that the outstanding material properties keep SiC devices advantageous over other available semiconductor devices in optical, high temperature, high frequency and high power applications (Atwell, 2002). It properties has made SiC a research focus till date (Zhao et al. 2020, Alkhalidi et al.2019 and Taylot et al. 2019)

This study started with calculating the lattice constant, band gap, plotting the band structure and plotting the density of states for cubic SiC. Then, SiC was doped with Boron and the changes after adding the impurity was observed by comparing the undoped and doped results. The modification in the band gap will affect or ensure the application of SiC.

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2. COMPUTATIONAL METHOD

Electronic structure calculations can be used to understand the electrical, optical, vibrational and thermal properties of materials under different physical and thermal conditions. First principle methods of calculations using density functional theory (DFT) are popular and dependable methods for studying properties of materials theoretically. We are using a first principle total energy code available for electronic structure calculations i.e., Biovia. Here the calculations are done using DFT with the local density approximation (LDA). Valence electrons are taken for calculations and the interaction between the valence electron and the cores is handled with the help of ab initio Vanderbilt pseudopotentials (Vanderbilt,1990). The calculations here are done using BIOVIA material studio. BIOVIA, a brand of Dassault Systems, is a scientific tool that can be used for research work. Biovia Materials Studio (Dahham et al. 2017) is a tool for modelling and simulation in Materials Science, Physics and Chemistry to study the structure and properties of materials under different conditions.

The cutoff values were taken as, kinetic energy cut off of 590.00 eV. A set of 2x2x2 or 1x2x2 or similar K-points scheme is used for BZ sampling. The exchange and correlation energy per electron is described by (Perdew and Zunger, 1981) parametrization of Monte Carlo calculations of (Ceperley and Alder, 1980) method. The single particle (Kohn and Sham, 1965) equations are solved and the eigen values are taken to interpret bulk band structure and the vacancy levels. The zinc blend crystal structure of SiC (Taylor and Laidler, 1950) is considered here for calculations. To begin with, the primitive unit cells with 2 atoms to make the computational calculation easier to handle. The lattice constant is expanded twice in all X and Y direction to create a supercell. Since we intend to do a doping of Boron in SiC so created a supercell of 32 atoms (16 Si atoms and 16 C atoms). One Boron atom is placed in place of Si atom. SO the percentage of impurity becomes 3.2%. Band energies were calculated for this supercell. The density of states was also plotted for this supercell.

The band energies, band plot and the density of states of undoped SiC and doped SiC with Boron are compared and presented here.

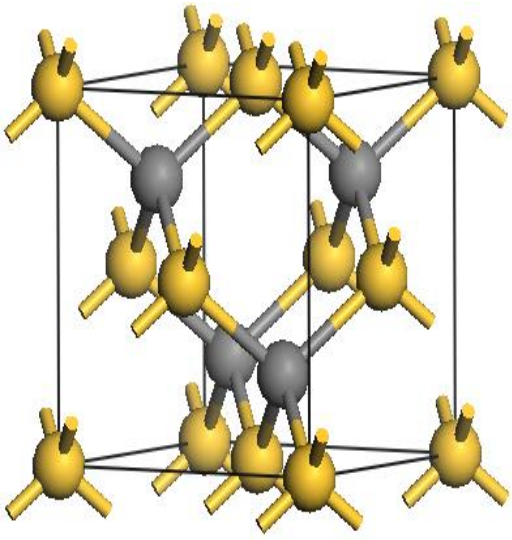

Figure 1: Crystal structure of SiC

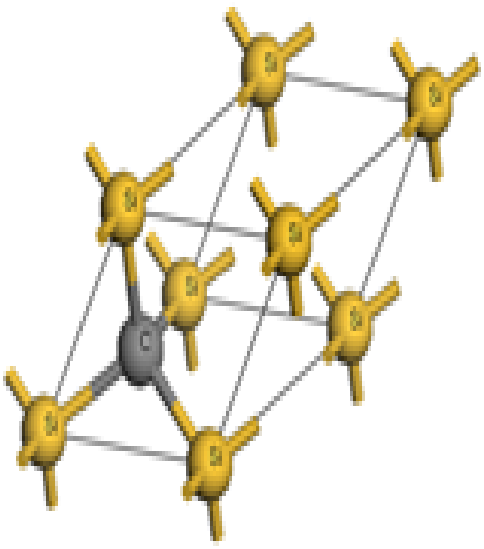

Figure 2: Primitive cell of SiC

Si in yellow and C in grey.

The calculations for the structural properties of the SiC was done taking a face centered cubic crystals and a primitive cell with 2 atoms in it. The cube taken into consideration having side '*a*', where *a* is the lattice constant. The primitive cell had 2 two atoms with Si at origin and C situated on the diagonal at a distance of 0.25 A. The primitive cell is shown in Fig. 2 and the BZ sampling is shown in Fig. 3. A supercell was created by expanding the lattice constant in the form 2x2x1 in X-, Y- and Z-direction. The corner Silicon atom is replaced with Boron atom. The new primitive cell contains total 32 atoms with 15 Silicon atoms, 1 Boron atom and 16 C atoms. The doped supercell is shown in Fig. 4. All calculations for doped case were done with this new primitive cell.

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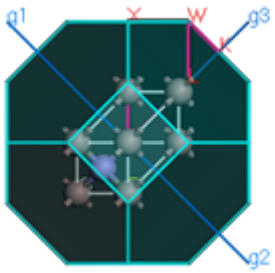

Figure 3: Brillouine zone of SiC

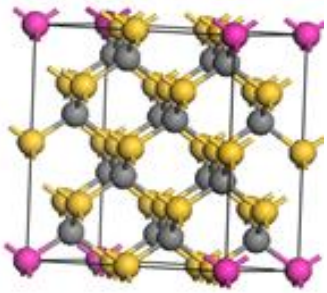

Figure 4: Boron doped SiC supercell. Yellow color represents Si atom, Grey is for C atoms and Pink is for Boron atoms.

3. RESULTS AND DISCUSSIONS

Density functional theory (DFT) (Hohenberg and Kohn, 1964) calculation for electronic properties of SiC were done. SiC crystalizes in zinc blende structure with primitive unit cells having 2 atoms. Calculations are carried out to find out the lattice constant of the primitive unit cell. These calculations require the determination of wave function and positions of all the valence electrons and 2 nuclei.

3.1 ELECTRONIC PROPERTIES

We started the calculation to find out the lattice constant for cubic SiC by energy minimization method. The lattice constant of a crystal corresponds to the size of the conventional unit cell and to obtain by plotting the total energy as a function of cell volume. Thus the calculated lattice constant for SiC is 3.0745A. The experimental lattice constant value for SiC is 4.359A. So our calculated value is in good agreement with the experimental value. The calculated energy band structure of SiC along direction of high symmetry is shown in figure 5. The top of the valence band is taken as ‘zero’ along the energy axis. The electronic configuration of Si is [Ne]3s2 3p2 and electronic configuration of C is [He]2s2 2p2. For this calculation, 3s2 3p2 electrons of Si and 2s2 p2 electrons of C were taken as the valence electrons. Use of smooth norm-conserving pseudopotential for Si and C helped in reducing the calculation effort.

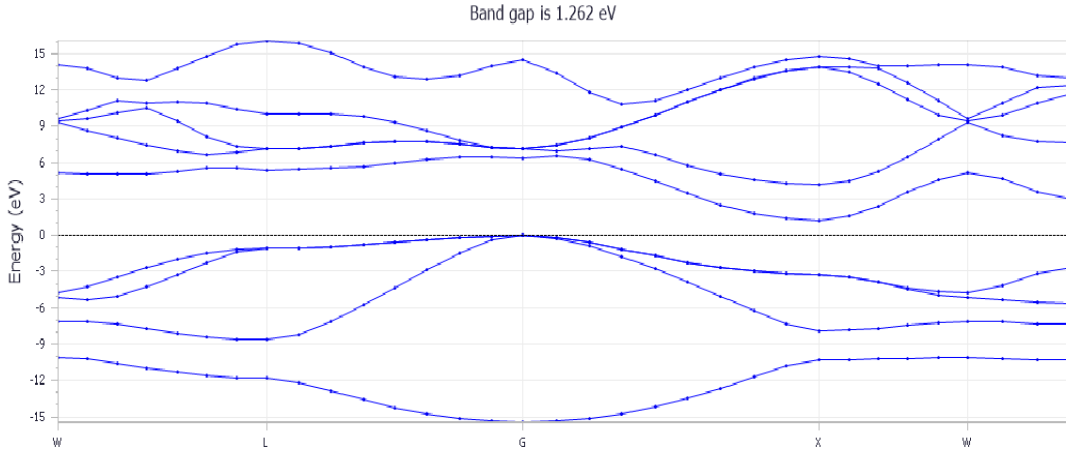

Fig 5 : Band structure of SiC for the primitive cell of two atoms. Top of the valence band is taken as zero on the energy axis.

The valence band maximum and conduction band minimum do not occur on the same symmetry line, indicating an indirect band gap. This is in accordance with published experimental results too (Baumeier et al. 2006) The calculated band gap is 1.325 eV. The experimental band gap of cubic SiC is 2.39 eV (Choyke et al. 1964) The smaller band gap compared to experimental value is due to the inherent drawbacks of LDA. Fig. 3.2 shows the band plot for SiC with 32 atoms in the primitive cell. More number of energy states are clearly visible owing to large number of atoms included in the calculations. However the band gap value remains the same. This also indicates an indirect band gap.

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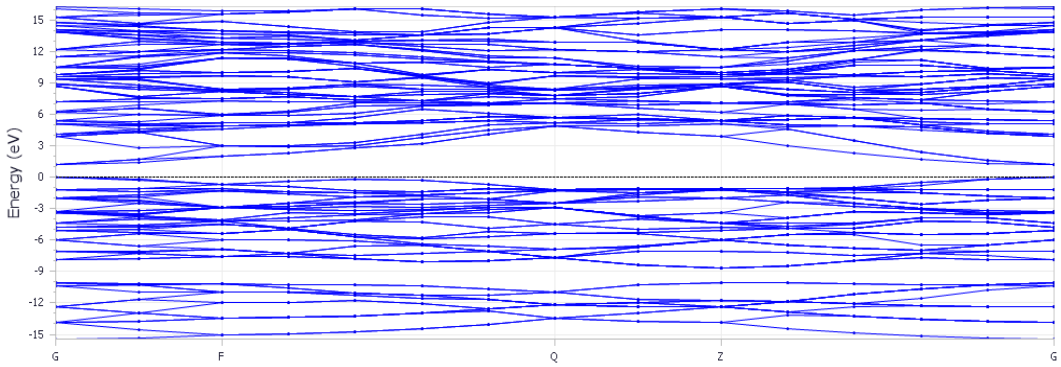

Fig 6 : Band structure of SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

The total density of states (DOS) of undoped SiC using first principle DFT with LDA using pseudopotential are shown in Fig. 7. Here the calculated densities of states are plotted against energy. The dotted line represents the Fermi energy. The left side of the line is the valence band and the right side represents the conduction band. The valence band has more number of electrons than the conduction band. This hence indicates the semiconducting behavior of SiC. The calculated density of states (DOS) was in nearly same to the previously reported DOS plot (Lu¨ning et al. 1999). The density of states plot given in Fig. 7 showed the many peaks but the maximum peak is at 8.2 eV.

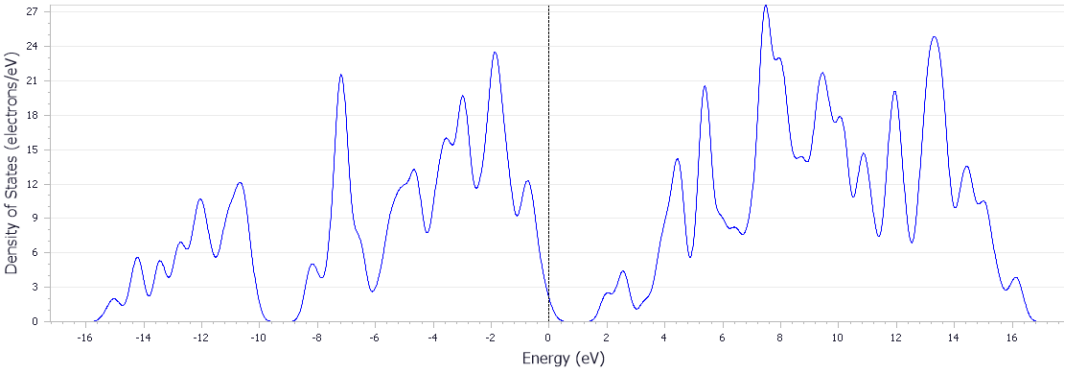

Fig 7: Density of states of SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

Fig. 8 shows the band energy plot for SiC doped with Boron in the supercell calculation. Comparing with the energy bands shown in Fig. 3.2, it is observed that the band gap remains the same before and after doping with Boron. But the indirect band gap of SiC has now changed to direct band gap. This indicates a change in the behavior of B doped SiC than pure SiC.

Fig. 9 shows the DOS plot for SiC doped with Boron in the supercell calculation. Comparing with the DOS plot shown in Fig. 7, it is observed that the band gap remains the same before and after doping with Boron. No significant change is observed in the Fermi energy level. The distribution of electrons in the valence and conduction band is also same in both undoped and doped cases.

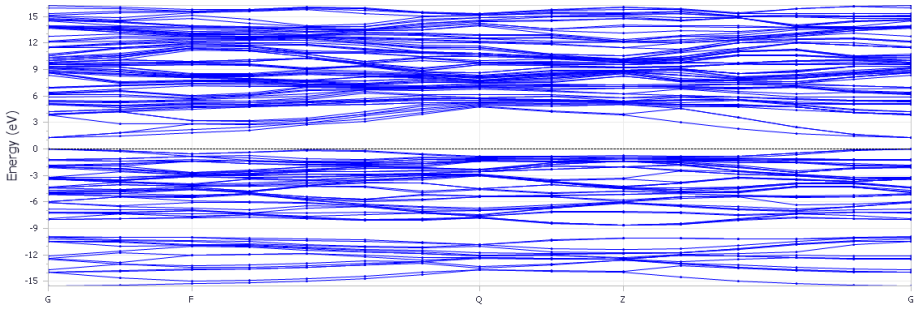

Fig 8: Band structure of Boron doped SiC for the primitive cell of 32 atoms. Top of the valence band is taken as zero on the energy axis.

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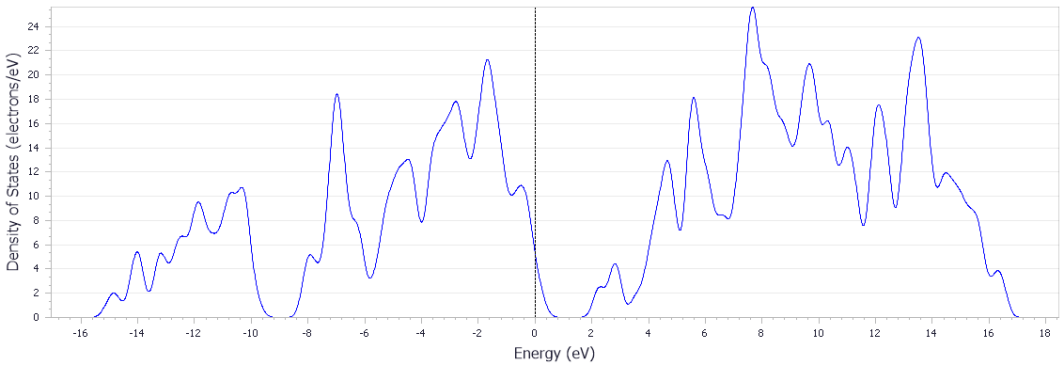

Fig 3 .5: Density of states of Boron doped SiC for the primitive cell of 32 atoms. Dotted line represents the Fermi energy.

4. CONCLUSIONS

The first principle DFT calculations to study the structural and electronic properties of cubic SiC was done. The values of lattice constant and band gap were found out. The band structure and density of states were plotted for SiC. All these were also done for SiC doped with Boron. The calculations were done using the Dassault system BIOVIA-Material Studio. Our observations can be summarized as follows.

The lattice constant of SiC is calculated with energy minimization method and found to be 3.0745A. The band gap was found out to be 1.325 eV. This value is less than the experimental value due to the use of LDA in this calculation. The band plot gave us information that SiC is an indirect band gap semiconductor. The energy band plot and DOS plot of SiC is compared with the respective plots for B doped SiC. The band gap remains the same before and after doping with Boron. But the indirect band gap of SiC has now changed to direct band gap. This indicates a change in the behavior of B doped SiC than pure SiC. This is an interesting result and it will be further interesting to verify the properties by increasing the percentage of doping.

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