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Ground State Electron Energies in sp_3 Hybridized Si and C Atoms in 4H-SiC Calculated from Ionization Energies

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Abstract:
In this research article, the ionization electron energies of sp3 hybridized Si and C atoms in 4H-SiC are calculated. The Si and C atoms are bonded tetrahedrally in 4H-SiC. The potential energy difference is found to be 0.13 eV from the ionization energies. The minimum number of Si-C bilayers are further calculated as 25 in 4H-SiC to give a theoretical bandgap of the bulk material as 3.25 eV, very close to the value of 3.26 eV calculated by applying the density functional theory.

Keywords: Bandgaps, Ionization, 4H-SiC, Composite semiconductor materials.

INTRODUCTION

4H-SiC semiconductor is technologically important semiconductor for high voltage power electronics applications with the advent of a power MOSFET such as a 650V MOSFET manufactured by the company called Infineon. This paper studies some relevant basic science of the 4H-SiC semiconductor material. Two recent articles by the author reports the minimum number of Si-C bi-layers needed in SiC semiconductor material so that the semiconductor exhibits the bulk semiconductor bandgap. The difference in the two papers is that the energy difference between the interacting electrons in the Si and C atoms of SiC are reported different. In one paper it is reported as 0.14 eV and in the other paper it is reported as 0.13 eV [1-2]. It needs to be stated that 0.13 eV is the correct energy difference and the calculation is shown in the present article starting from the ionization energy formula.

THEORY

SiC polytypes have different stacking sequence of the tetrahedrally bonded Si-C bilayers such as 3C-SiC has the sequence of ABCABC... of three positions with respect to the lattice denoted as A, B, and C. Similarly, 2H-SiC has the sequence ABAB..., 4H-SiC has the sequence ABCBABCB...., with 4 layers repeated, and 6H-SiC has the sequence ABCACBABCACB..., with 6 layers repeated. The ground state energy levels of the interacting electrons of a Si and C atom in SiC has shown a difference of 0.13 eV in energy [3]. This energy difference can be calculated from the ionization energies of electrons in Si and C atoms forming tetrahedral bonds with the sp^3 hybridized bonds in both Si and C. The formula for the ionization energy of an atom is given as:

$$E_n = -13.6 \times n^2/Z^2 \text{ in eV/atom,}$$

where n is the shell number in the atomic configuration and Z is the atomic number of the atom.

RESULTS AND DISCUSSIONS

The ionization energies for 4 electrons and one electron in Si and C atoms is calculated utilizing the formula for ionization energy presented in the theory section. The results are tabulated below

Table 1. Ionization energies of electrons in Si and C atoms

Elements	Atomic Number, Z	Shell Number, n	Ionization Energies of 4 electrons in eV	Ionization Energies of 1 electron in eV
Si	14	3	- 0.6244	- 0.1561
C	6	2	- 1.5111	- 0.3777

Furthermore, the p-orbital after sp^3 hybridization in C atom changes the angle from 90^o to 109.47^o. The change in angle is 19.47^o. Therefore, the ionization energy of the electron of the sp^3 orbital increases by -0.3777/Cos (19.47^o) =- 0.40 eV as the potential energy of one electron of the C atom at the corner of the unit cell. To form the sp^3 tetrahedral bond in 4H-SiC for example, the orbital lies along the body diagonal of the unit cell of size 2, from the centre having Si atom to the corner having C atom. The p-orbital after hybridization reduces in size causing the Coulombic force between the two interacting electrons to increase. The work done is force times the distance. Therefore, the energy of the electron therefore increases by the factor of the body diagonal of $\sqrt{3}$. Assuming a bond with Si at the centre and the C at the corner makes the energy of the Si sp^3 electron as -0.1561 x $\sqrt{3}$ = -0.270 eV as the potential energy of one electron of the Si atom at the centre. The difference in the sp^3 electron energies becomes -0.27- (-0.40) = 0.13 eV [3].

It can be calculated that the minimum number of Si-C bilayers with this energy difference of 0.13 eV will be 25 for the 4H-SiC to give the theoretical bandgap of 0.13 x 25 = 3.25 eV [1-2]. The study utilizing the density functional theory reports a value of 3.26 eV as the bandgap of 4H-SiC [4]. The experimental bandgap of 4H-SiC is reported as 3.23 eV [5].

CONCLUSION

The ionization energies as the potential energy of one electron each in the Si and C atom of tetrahedrally bonded 4H-SiC are -0.27 eV and -0.40 eV respectively after sp^3 hybridization of both the atoms and forming the tetrahedral bond. The minimum number of Si-C bilayers in 4H-SiC semiconductor are calculated to be 25, to give a theoretical bandgap of 3.25 eV. The method could be applied to other composite semiconductor materials, and could form a new method to find the bandgap of a semiconductor.

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