

# Minimum Number Of Si-C Bilayers Needed In Polytypes Of Sic Semiconductor To Exhibit Bandgaps Of Bulk Materials

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## **Abstract:**

*In This Research Article, The Minimum Number Of Si-C Bilayers Needed In Polytypes Of Sic Semiconductor Are Calculated, Such That The Semiconductor Materials Exhibit Bandgap Of Bulk Materials.*

**Keywords:** *Bandgaps, Sic, MOS Device, Composite Semiconductor Materials.*

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## **I. Introduction**

An excellent review article on wide bandgap semiconductors is written by Morkoc et al., which describes the physics and chemistry of large bandgap semiconductor materials technologically important for electronic and optical applications of the future [1]. The author has in this article chosen to highlight a simple method to bring about the science regarding the SiC polytypes that can ease research in wide bandgap materials composed of two elements in place of one, such as SiC and GaN. Science on other composite semiconductor materials can also be uncovered with the help of the present research.

## **II. Theory**

Different 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 ABCBABC..., with 4 layers repeated, and 6H-SiC has the sequence ABCACBABCACB..., with 6 layers repeated. The ground state energy levels of a Si and C atom in SiC has shown a difference of 0.13 eV in energy [2]. This energy difference can be used to calculate the minimum number of Si-C bilayers needed for the SiC semiconductor polytypes to exhibit their bulk bandgaps.

## **III. Results and Discussion**

The author has recently found the conduction band offset (CBO) in an n-type 4H-SiC Metal-Oxide-Semiconductor (MOS) device oxidized on the Carbon face of the (000-1) oriented 4H-SiC surface. It came out to be 2.92 eV [3]. It has also been confirmed by Nemoto et al. utilizing an n-type 4H-SiC MOS device oxidized on the Si-face and having a Ni gate, where the valence band offset (VBO) on the n-type 4H-SiC MOS device oxidized on the Si-face is the CBO on the n-type 4H-SiC MOS device oxidized on the C-face [3-4]. The CBO on the n-type 4H-SiC MOS device oxidized on the Si-face of the (0001) oriented 4H-SiC surface was already known to have a truncated value of 2.78 eV and a rounded value of 2.79 eV, also characterized by the author [5-6]. The difference in the two band offsets gives the energy difference between the ground states of the Si and C atoms in SiC semiconductor polytypes as  $2.92 - 2.79 = 0.13$  eV utilizing the rounded value of CBO of 2.79 eV in place of the truncated value of 2.78 eV. The truncated value of 2.78 eV gives the energy difference of 0.14 eV [3]. In this research paper the 0.13 eV energy difference between the ground states of the Si and C atoms in SiC is used to calculate the minimum number of Si-C bilayers required for different polytypes of SiC to exhibit their bulk bandgaps. The results are presented in Table 1 below where the minimum number of bilayers and the theoretical bandgaps are presented in columns 4 and 5. For example, the minimum number of bilayers for the 4H-SiC are 25 formed out of 26 layers starting with Si layer and ending with a Carbon layer, and giving a theoretical bandgap of  $0.13 \times 25 = 3.25$  eV. The reported theoretical bandgap of bulk 4H-SiC based on density functional theory (DFT) calculations is 3.26 eV [7]. The experimental bandgap of 4H-SiC is reported as 3.23 eV. Thus, the DFT calculations of the bandgaps can be compared to the one obtained by the method presented in this research paper.

It is known that the experimentally obtained bandgap of 2H-GaN is 3.39 eV close to that of 4H-SiC at 3.23 eV. The closest number of Ga-N bilayers for the wurtzite 2H-GaN will be 26, given the same energy

difference in the ground states of Gallium and Nitrogen atoms of 0.13 eV. This shows that 0.13 eV could be the energy difference between the ground states of Ga and N atoms in 2H-GaN also, or very close to it. For the zincblende 3C-GaN, the minimum number of Ga-N bilayers could be 25, given that the experimental bandgap is 3.2 eV as observed and reported.

**Table I. Calculated minimum number of Si-C bilayers in SiC polytypes and their bandgaps**

S.No.	Semiconductor Polytype	Ground State energy difference between Si and C atoms in SiC (eV)	No. Of Bilayers of Si-C	Theoretical bandgap of bulk SiC (eV)	Reported experimental bandgap, (eV)
1.	4H-SiC	0.13	25	3.25	3.23
2.	6H-SiC	0.13	23	2.99	3.02
3.	3C-SiC	0.13	18	2.34	2.38
4.	2H-SiC	0.13	26	3.38	3.33
5.	15R-SiC	0.13	23	2.99	3.0

#### IV. Conclusions

The minimum number of Si-C bilayers in SiC semiconductor polytypes are calculated easily with the known experimental bandgap and the energy difference in the ground states of Si and C atoms in SiC, using simple arithmetic. They are presented in a Table above. For example, the number of bilayers for 4H-SiC are 25 and the theoretical bandgap of 4H-SiC is 3.25 eV. The energy difference in the ground state of the Ga and N atoms in GaN could also be very close to 0.14 eV. The method could be applied to other bi-layer containing composite semiconductor materials.

#### References

- [1]. H. Morkoc, S. Strite, G.B. Gao, M.E. Lin, B. Sverdlov, And M. Burns, "Large-Band-Gap Sic, Iii-V Nitride, And Ii-Vi Znse-Based Semiconductor Device Technologies", *Journal Of Applied Physics*, 1994;76(3):1363-1398.
- [2]. J. Borysiuk, J. Soltys, R. Bozek, J. Piechota, S. Krukowski, W. Strupinski, J.M. Baranowski, R. Stepniewski, "Role Of Structure Of C-Terminated 4h-Sic (000-1) Surface In Growth Of Graphene Layers: Transmission Electron Microscopy And Density Functional Theory Studies", *Arxiv.Org, Cornell University Run Website*, 2011.
- [3]. R.K. Chanana, "Computation And Confirmation Of Conduction Band Offset And Oxide Breakdown Fields From A Combination Of Electrical And Physical Measurements On An N-Type C-Face 4h-Sic Mos Device", *Iosr-Journal Of Electrical And Electronics Engineering*, 2020;15(1):1-6.
- [4]. H. Nemoto, D. Okamoto, X. Zhang, M. Sometani, M. Okamoto, T. Hatakeyama, S. Harada, N. Iwamuro, H. Yano, "Conduction Mechanisms Of Oxide Leakage Current In P-Channel 4h-Sic Mosfets", *Jpn. J. Applied Phys.*, 2020;59(4):044003.
- [5]. R.K. Chanana, K. Mcdonald, M. Diventra, S.T. Pantelides, L.C. Feldman, G.Y. Chung, C.C. Tin, J.R. Williams, R.A. Weller, "Fowler-Nordheim Hole Tunnelling In P-Sic/Sio<sub>2</sub>, Structures", *Appl. Phys. Letts*. 2000;77(16):2560-2562.
- [6]. R.K. Chanana, "Determination Of Hole Effective Mass In Sio<sub>2</sub> And Sic Conduction Band Offset Using Fowler-Nordheim Tunnelling Characteristics Across Metal-Oxide-Semiconductor Structures After Applying Oxide Field Correction", *J. Appl. Phys.*, 2011;109:104508-1 To 6.
- [7]. A.V. Sinelnik, A.V. Semenov, "Theoretical Study Of The Band Structure Of 2h-Sic And 4h-Sic Of Silicon Carbide Polytypes", *Condensed Matter Physics*, 2021;24(2):23706-1 To 6.