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SERVICES FOR SCIENCE AND EDUCATION

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 short 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, Bilayers, Semiconductors, Materials.

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.

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 ABCBABCB…., with 4 layers repeated, and 6H-SiC has the sequence ABCACBABCACB…, with 6 layers repeated. The ground state energy levels of a Si and Carbon atom in SiC has shown a difference of 0.14 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.

RESULTS AND DISCUSSIONS

The author has used the ground state energy difference of 0.14 eV between the Si and C atoms in SiC semiconductor to find out the conduction band offset in 4H-SiC MOS device oxidized on the Carbon face and oriented in the (000-1) direction. The conduction band offset comes out to be 2.92 eV for C-faced 4H-SiC-MOS device [3]. In this research paper the 0.14 eV energy difference 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 3 and 5. For example, the minimum number of bilayers for the 4H-SiC are 23 formed out of 24

layers starting with Si layer and ending with a Carbon layer, and giving a theoretical bandgap of 0.14 x 23 = 3.22 eV. The experimental bandgap of 4H-SiC is known to be 3.23 eV.

Table 1. Calculated minimum number of Si-C bilayers in SiC polytypes and their bandgaps

S.No.	Semiconductor Polytype	No. Of Bilayers of Si-C	Ground State energy difference between Si and C atoms in SiC (eV)	Theoretical bandgap (eV)	Experimental bandgap, (eV)
1.	3C-SiC	17	0.14	2.38	2.38
2.	2H-SiC	24	0.14	3.36	3.3
3.	4H-SiC	23	0.14	3.22	3.23
4.	6H-SiC	21	0.14	2.94	3.02

It is known that the experimentally obtained bandgap of 2H-GaN is 3.39 eV. The closest number of Ga-N bilayers for 2H-GaN will be 24, given the same energy difference in the ground states of Gallium and Nitrogen atoms of 0.14 eV. This shows that 0.14 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 3C-GaN, the minimum number of Ga-N bilayers could be 23, given that the experimental bandgap is 3.2 eV as observed and reported.

CONCLUSION

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 23 and the theoretical bandgap of 4H-SiC is 3.22 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.

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