

Full Length Research Paper

First principles studies of band structure calculations of 6H-SiC and 4C-SiC using pseudopotential approaches

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We have studied the band structure properties of SiC in wurtzite and zincblende crystal structures. In our calculations, we have adopted a pseudopotential approach based on the Density Functional Theory (DFT). We have calculated the band structure and density of state (DOS) and therefore, the changes of the energy gap of this compound with crystal structure. The quality of the used pseudopotential was tested by comparing the calculated band structure and DOS, using Full Potential Linear Augmented Plane Wave (FP-LAPW) and pseudopotential methods. The result shows that, the electronic band structure and density of state data for SiC in wurtzite and zincblende crystal structures are comparable with their experimental calculations. It was also found that both structures are direct band gap semiconductor centered at the Γ point.

Key words: Pseudopotential, Density Functional Theory, augmented plane wave.

INTRODUCTION

SiC is a wide band gap semiconductor and therefore has a lot of applications in high-temperature and high power device industry. These properties combined with good thermal conductivity and stability makes SiC an attractive material for fabrication devices and radiate harsh environment electronic devices (Look et al., 1998). It has been shown that, SiC has large peak electron velocity and can be an important candidate for high frequency application (Makino et al., 2001).

A wide energy band gap leads to a low intrinsic carrier concentration, which enables a more precise control of free carrier concentration, over a wide range of carrier concentration over a wide range of temperatures (Chen et al., 1998) and hence, the devices made of this kind of material will be operable at high temperatures, with large breakdown voltage (Mansour et al., 1991). The development of SiC and based transport devices is hampered by the nonavailability of detailed knowledge of the band structure parameters (Brennan, 1998). Keeping in mind its huge technological prospect, we need a better understanding of this material (Chattopadhyay and Queisser, 1981). 6H-SiC (wurtzite crystal structure) is believed to be the most important SiC polytype in

comparison to 4C-SiC (zincblende crystal structure) for high reliability power field effect transistor technology due to the higher conduction band offset with SiO₂ (Di and Brennan, 1991).

In this paper, we report a calculation which is used to model band structure in hexagonal and cubic SiC. Here, we have employed the pseudopotential approaches based on the density functional theory. Details of the employed model is presented next. This is followed by the results of the band structure calculations carried out on wurtzite and zincblende; then, SiC crystal structures are interpreted subsequently.

Model details

First principles or ab-initio approaches provide a method for modeling systems based solely on their atomic coordinates and the Z numbers of the different atoms. These techniques rely on the fact that, there should be one unique charge density or distribution which describes the ground state of a system. This reduces the problem of solving for the electronic structure of a system, from a 3N dimensional problem to one that only depends on the charge density. A number of approaches have been developed to properly reduce a system to the minimum energy electronic configuration and abinit includes several of these (Gonze et al., 2002). First principles codes such as abinit have proved useful to topics ranging from the composition of the planetary core to the electrical properties of single molecules (Kohn and Sham, 1965). Abinit can

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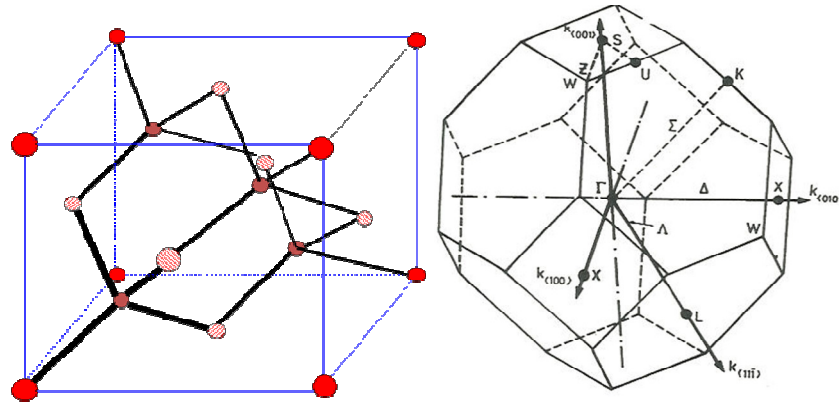


Figure 1. The crystal structure of zincblende 4C-SiC and the first Brillouin zone of a zincblende crystal with the principal symmetry directions and points.

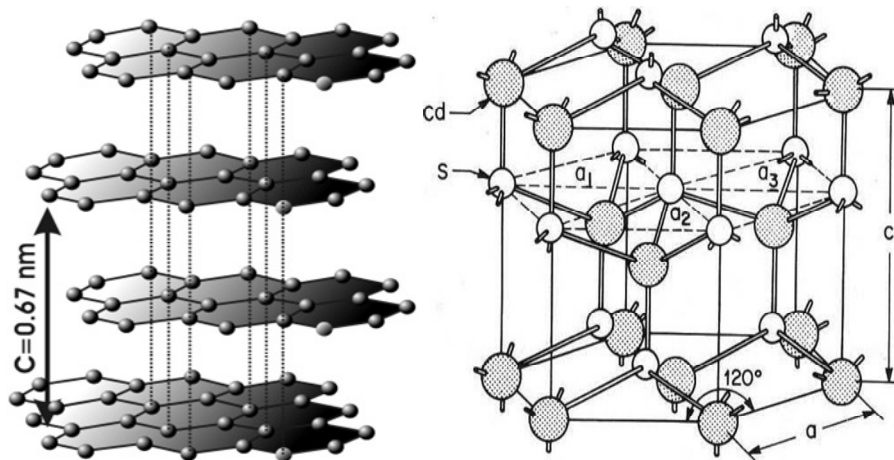


Figure 2. The crystal structure of wurtzite 6H-SiC and the first Brillouin zone of a wurtzite crystal with the principal symmetry directions and points.

calculate the forces on atoms in a structure and use this information to relax the system. This has provided critical understanding in how surfaces reconstruct, how adsorbates interact with surface sites, and how magnetic impurities affect neighbor lattice sites. Typically, calculations can consider 30 to 40 atoms comfortably. Larger systems can be done, but for fairly large systems (greater than 150 atoms), parallel calculations are essential (Hohenberg and Kohn, 1964).

In addition to minimizing the total energy of a structure, abinit can also calculate band structures, density of states, magnetic properties, and phonon dispersion curves. We made a $6 \times 6 \times 6$ super cell of the unit cell which contain 48 atoms and then substituted some of the Si atoms by C atoms in wurtzite or zincblende crystal structures. There are two important parameters which should be optimized correctly for saving time and also to have an acceptable precision in calculations. These parameters are cutoff-energy and kgrid-cutoff, where their optimized values were chosen.

SiC can crystallize in either the zincblende or wurtzite structures, which have slightly different material properties and substantially different band structures. However, the wurtzite phase of SiC is the more stable bulk form of the material and the common form for epitaxial layers, although thin epitaxial layers can be grown with the

zincblende structure. SiC in the zincblende structure is shown in Figure 1. It can be regarded as two interpenetrating face-centred cubic (fcc) Bravais lattices, displaced along the diagonal of the cube in Figure 1a by one quarter of its length. Si atoms are located on one fcc lattice and C atoms on the other resulting in a structure where each atom is surrounded by four neighbors of the other type at the corners of a regular tetrahedron. Figure 1 shows also the first Brillouin zone of SiC in the zincblende structure. The first Brillouin zone is a truncated octahedron of volume $4(2\pi/a)^3$. It has 14 faces, six squares perpendicular to the (100) directions and eight regular hexagons perpendicular to the (111) directions. The high-symmetry points Γ , X and L, which are at the centre of the Brillouin zone, the centers of the squares and the centers of the hexagons respectively, are indicated in the figure. The wurtzite crystal structure of SiC is shown in Figure 2.

It can be regarded as an interpenetration of two hexagonally close packed (HCP) sub-lattices with a relative displacement along the c-axis by u where u is the so called internal parameter and c is the lattice constant for the c-axis. The distance between in-plane atomic neighbors is denoted by a . For an ideal wurtzite structure $c/a = (8/3)^{1/2} = 1.633$ and $u = 3/8 = 0.375$ and the atoms have the regular tetrahedral coordination of nearest neighbors that occurs for

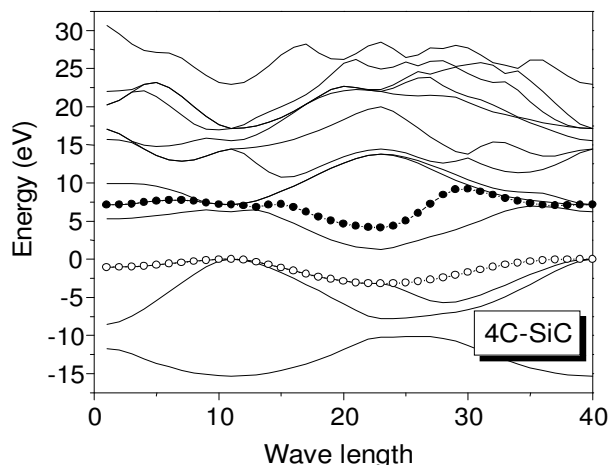


Figure 3. The band structure of zincblende SiC in the main directions of symmetry calculated from pseudopotential theory.

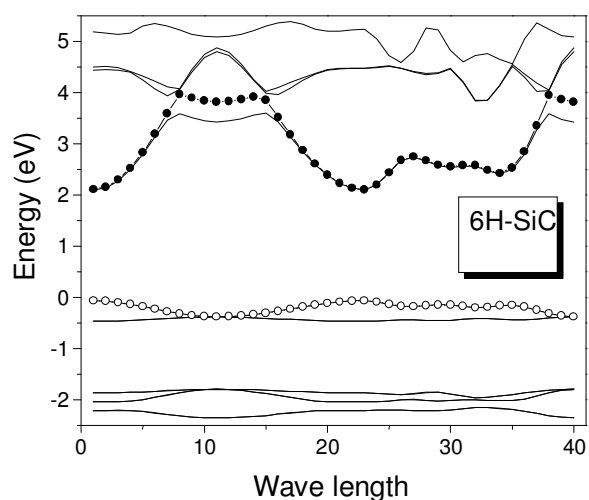


Figure 4. The band structure of wurtzite SiC in the main directions of symmetry calculated from pseudopotential theory.

the zincblende structure. The difference between the two structures is in the next nearest neighbor arrangement. The first Brillouin zone of wurtzite SiC which is a hexagonal prism of volume is shown in Figure 2 as well, together with the locations of the high-symmetry points Γ , K, M and U.

RESULTS AND DISCUSSION

The calculated band structures for SiC in zincblende and wurtzite crystal structures have been shown in Figures 3 and 4. It is evident that both semiconductors are direct band gap at the Γ point. The obtained band gap for 4C-SiC is about 2.1 eV whereas for 6H-SiC it is about 3 eV. It

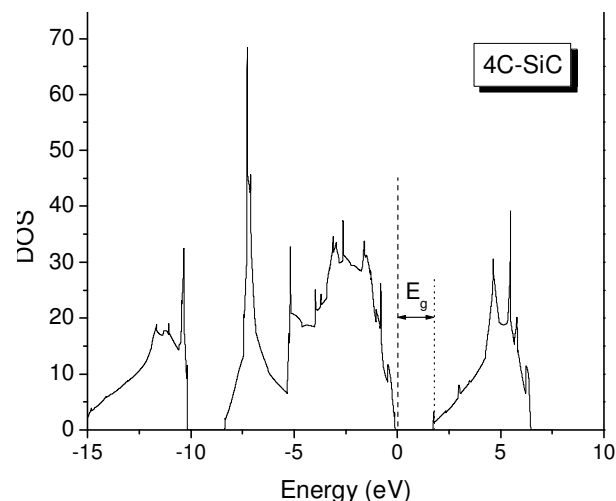


Figure 5. The calculated total density of states in 4C-SiC.

can be seen from Figures 3 and 4 that, although the band structures of the two phases of SiC have some similarities (both have direct fundamental gaps at the Γ point that differ by only about 10%, the conduction bands are sufficiently different to cause a significant variation in their electron transport properties.

For example, the nearest satellite valley in the zincblende structure (X point) is about 1.5 eV above the lowest conduction band minimum while the nearest satellite valley in the wurtzite structure, at the U point, is about 2 eV above the minimum. Also, in the wurtzite SiC band structure, there is a second Γ conduction band valley at a relatively low energy, approximately 2.1 eV above the lowest minimum valley. The total density of state of 4C-SiC between -15 and 7 eV is shown in Figure 5. There are a large number of relatively localized states at the top of the valance band, originating mainly from the Si to C atoms. The valance band edges near the Fermi energy for Si atom are quite sharp, while the conduction band edges near the Fermi energy are not. The valance band, which lies between 0 eV (Fermi energy) to -10 eV, is composed of the 2p orbital hybridized d orbital. The lower valance is formed predominantly by Si 2s atom and extends from -10 to -15 eV.

The total density of state of 6H-SiC has been shown in Figure 6. By comparing Figures 5 and 6, it can be seen that with changing crystal structure from zincblende to wurtzite results in increasing the band gap. In wurtzite crystal structure of SiC the number of localized states at the top of the valance band shifts from -15 eV to -3 eV. The band gap increases mainly due to the number of states originating from d-state in the conduction band.

Conclusions

In conclusion, we have studied the band structure and

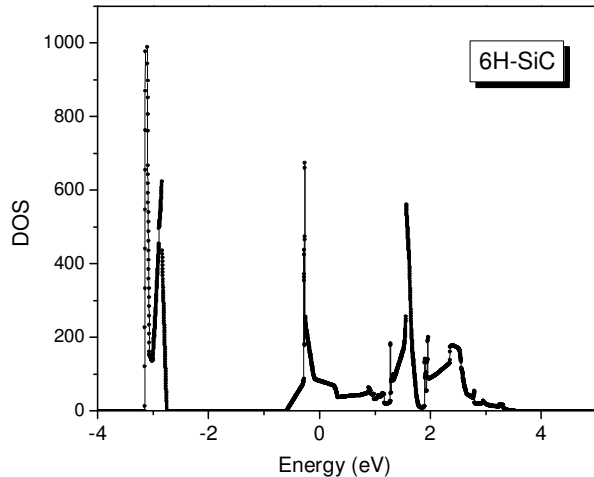


Figure 6. The calculated total density of states in 6H-SiC.

density of state in 4C-SiC and 6H-SiC crystal structures from the first principle method. From these results, we showed that both phases of SiC semiconductor are direct band gap materials and wurtzite phase has a larger band gap.

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