Electronic structure and charge transfer in 3C- and 4H-SiC

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Abstract. We utilized a local density functional potential, the linear combination of atomic orbital (LCAO) method, and the BZW procedure to study the electronic structure of 3C- and 4H-SiC. We present the calculated energy bands, band-gaps, effective masses of n-type carriers, and critical point transition energies. There is good agreement between the calculated electronic properties and experimental results. Our preliminary total energy calculations for 3C-SiC found an equilibrium lattice constant of $a = 4.35$ Å, which is in agreement with the experimentally measured value of 4.348 Å. The calculated charge transfers indicate that each silicon atom loses about 1.4 electrons that are gained by a carbon atom in both 3C- and 4H-SiC.

1. Introduction

Due to its superior electronic, mechanical and chemical properties, silicon carbide (SiC) has become one of the most promising materials for high-temperature and high-power device applications [1, 2]. The large Si-C bonding energy makes SiC resistant to chemical attack and radiation and ensures its stability at high temperature. SiC is probably the most prominent material that exhibits a wide range of polytypism. More than 200 SiC polytypes have been determined. Among the SiC polytypes, 3C and 4H polytypes are attracting more attention for their favourable electronic properties.

In this paper, we report ab initio studies of the electronic structure and charge transfer in 3C- and 4H-SiC. Ab initio approaches based on density functional theory, in the local-density approximation (LDA) [3, 4], are well established as very powerful tools for studying properties of semiconductors, metals, surfaces, or interfaces [5, 6, 7, 8, 9]. In these ab initio calculations, the exchange–correlation interactions for the many-body electron system are expressed as a functional of the electronic charge density [3, 4, 5].
However, many LDA calculations for semiconductors or insulators often underestimated the band-gaps by 30–50%. Closely related to the band-gap problem, the calculated low energy conduction bands and optical properties of semiconductors—from many LDA computations—also disagree with experimental results. In the case of previous LDA calculations for Ge, several theoretical band structures are metallic [8, 10, 11], in contrast to experimental results. There have been some theoretical efforts intended to address these issues, including calculations that utilize nonlocal, energy-dependent, non-Hermitian self-energy operators [12, 13, 14, 15, 11]. Aryasetiawan and Gunnarsson reviewed several computational approaches, including the GW method, aimed at describing excited state properties [16]. These authors have shown that with converged basis sets and improved exchange and correlation, the calculated band-gap becomes generally correct. Johnson and Ashcroft utilized some simplified applications of the GW method to make scissors-type corrections to the band-gaps of semiconductors [17].

In previous reports [18, 19], Bagayoko and co-workers identified an effect inherent to the variational calculations that utilize a basis set, as done in the LCAO method. This effect is concomitantly due to basis sets and to intrinsic properties of the Rayleigh–Ritz variational approach as explained below. The Rayleigh theorem [20, 23] states that when an eigenvalue equation is solved by the LCAO method, using a basis set of \( N \) orbitals and one of \((N + 1)\) orbitals, where the larger set of size \((N + 1)\) is obtained by augmenting the smaller one of size \( N \), then the calculated eigenvalues satisfy the following inequalities:

\[
E_N^1 \geq E_1^{N+1}, \quad E_N^2 \geq E_2^{N+1}, \quad E_N^3 \geq E_3^{N+1}, \quad \ldots
\]

Succinctly, and provided the above conditions are met, a given eigenvalue is never increased by an increase of the size of the basis set; it either remains unchanged (i.e. if it is equal to the exact value) or is lowered to approach the exact eigenvalue from above. This theorem clearly dictates the use of large basis sets to ensure the convergence of calculated eigenvalues to the corresponding exact ones. Further, completeness consideration requires that the basis sets be as large as possible. Consequently, variational calculations generally place a needed emphasis on ensuring convergence by utilizing large basis sets. The method described below recognizes this requirement and the fact that only the wavefunctions of occupied states are used in the iterative procedure to reconstruct the charge density and the potential. This last fact provides a possible criterion for determining an optimum basis set, i.e., the convergence of the eigenvalues of all the occupied states. This criterion essentially defines the Bagayoko, Zhao and Williams (BZW) procedure that adds to the available approaches for first-principle calculations of properties of materials, with emphasis on the description of excited states and band-gaps.

This procedure has been applied to describe, within the local density approximation, the electronic and optical properties of BaTiO\(_3\) [19], wurtzite GaN, Si, diamond (C) and RuO\(_2\) [24]. In this paper, we report our calculations of the electronic properties and charge transfer for 3C- and 4H-SiC, employing the BZW procedure [18, 19, 24].

In the next section, we summarize our computational method. The calculated results are presented in section 3. They are followed by a short conclusion in section 4.

2. Method

Our self-consistent calculations utilized the \( ab\, initio \) linear combination of atomic orbital (LCAO) method. These self-consistent LCAO calculations included all electrons and full potentials, without shape approximations. Details of the general computational method are available in previous publications [7, 25, 26, 27, 28, 29]. We employed the Ceperley–Alder type [30] of the local density functional potential as parametrized by Vosko \( et\, al \) [31]. The newly developed BZW
procedure [18] is employed throughout the calculations. Our calculations are non-relativistic.

Bagayoko, Zhao and Williams (BZW) utilized the criterion discussed above to introduce an \textit{ab initio} procedure for identifying optimal basis sets in variational calculations. Essentially, this procedure requires the performance of three or more self-consistent calculations, beginning with the minimal basis set. The minimal basis set is that required to account for all the electrons of the atomic or ionic species in the material (molecules, clusters, or solids). Every subsequent calculation is carried out with a basis set including that for the previous calculation plus one (or more) orbital of the atomic or ionic species that are present in the material under study. These orbitals are added in the order of increasing energy. Several self-consistent calculations are done until the energies of the occupied states, for calculation \( N \), are the same as those for calculation \( (N + 1) \). Then, the material is studied using the basis set from calculation \( N \), known as the optimum basis set. Physically, the BZW procedure defines a new form of convergence, i.e. that of the occupied states (or charge density) with respect to the size of the basis set.

In these calculations for 3C- and 4H-SiC, the atomic wavefunctions were constructed from results of self-consistent \textit{ab initio} atomic calculations. The radial parts of the atomic wavefunctions were expanded in terms of Gaussian functions. Even-tempered sets of Gaussian exponents were employed for both Si and C. The minimum and maximum Gaussian exponents for Si are 0.16 and 0.65 \( \times 10^5 \), in atomic units, respectively. The minimum and maximum exponents for C are 0.1 and 0.65 \( \times 10^5 \). We included 22 Gaussian orbitals for the expansion of the atomic wavefunctions of the s and p states for Si and C. For the extra atomic wavefunction of Si(3d), we used 18 Gaussian orbitals. We found that the optimal basis set [18, 19, 24] for the LCAO calculations of the electronic structures of 3C- and 4H-SiC consists of the atomic orbitals of Si(1s2s3s4s 2p3p 3d) and C(1s2s3s 2p). Here, Si(4s 3d) and C(3s) represent empty shells in free atoms or ions. They are used to augment the basis set to account for charge redistribution in the solid environment.

3C-SiC (or \( \beta \)-SiC) is the only type of the cubic structure of silicon carbide with a zinc-blende arrangement. In our studies of the electronic structure of 3C-SiC, we used a lattice constant of \( a = 4.35 \) Å, which is the experimentally measured value. Our calculations of the total energy led to this value as the theoretical one. In the self-consistent calculations of 3C-SiC, we included 28 general \( k \)-points in the irreducible Brillouin zone, with proper weights. The computational error for the valence charge was about 0.00056 for 16 electrons. The self-consistent potential converged to about \( 10^{-5} \).

4H-SiC belongs to the \( C_{6v}^4 \) group. The atoms of its four ‘molecules’ are all on the trigonal axes in the special positions of the \( C_{6v}^4 \) group:

\[
\begin{align*}
(2a) & \quad (0, 0, u); (0, 0, u + 1/2); \\
(2b) & \quad (1/3, 2/3, v); (2/3, 1/3, v + 1/2)
\end{align*}
\]

with \( u(\text{Si}) = 3/16 \), \( v(\text{Si}) = 7/16 \), and \( u(\text{C}) = 0 \), \( v(\text{C}) = 1/4 \). We used the experimental lattice constants of \( a = 3.073 \) Å, and \( c = 10.053 \) Å. In the self-consistent calculations of 4H-SiC, we included a mesh of 24 \( k \)-points, with proper weights, in the irreducible Brillouin zone. The computational error for the valence charge was about 0.25 for 64 electrons. The self-consistent potentials converged to a difference around \( 10^{-5} \) after about 50 iterations. The total number of iterations varies with the input potentials.
3. Results

3.1. Electronic structure and total energy of 3C-SiC

The electronic energy bands of 3C-SiC, calculated with the optimal basis set, are shown in figure 1. The zero of the energy is set at the top of the valence band. The top of the valence band of 3C-SiC is at the $\Gamma$-point and the lowest conduction band is at the X-point. Our calculated valence bands of the occupied states of 3C-SiC, figure 1, are very close to the previously reported results of \textit{ab initio} LDA calculations [11, 33, 34, 35, 36, 37, 38]. Such agreements are expected from the BZW procedure, since the optimal basis set is the smallest basis set that leads to the same occupied eigenvalues or charge density as all the larger basis sets. The extra lowering of the unoccupied states of the conduction bands, as noted above, is avoided methodologically by the BZW procedure. Comparing our calculated conduction bands in figure 1 with previously reported results for 3C-SiC shows differences that are not a rigid shift of a set of bands with respect to another. These differences between our calculated conduction bands and previous LDA results directly affect the band gap and electron transition energies. Our calculated indirect band-gap of 3C-SiC is 2.24 eV, which is very close to the experimental value of about 2.2–2.4 eV [1, 32]. The previous LDA calculations obtained a theoretical band-gap of about 1.3 eV [33, 11], which was much smaller than experimental results.

Table 1 lists our calculated critical point transition energies of 3C-SiC, along with experimental results. In this table, the indexes v and c refer to the valence and conduction bands, respectively. The experimental transition energies are deduced from the decomposition analysis of the $\epsilon_2(\omega)$ spectrum [41]. Our calculated optical transitions, without any shift, agree well with experimental results. The previously calculated critical point transition energies of 3C-SiC differ with experimental results by about 1 eV [41]. We ascribe the difference between previous LDA results and experiments to the effect circumvented by the BZW procedure as noted above.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{energy_bandstructure.png}
\caption{The calculated electronic energy band structure of 3C-SiC along high-symmetry directions, as obtained with the optimal basis set from the BZW procedure.}
\end{figure}
Table 1. Comparison of the calculated critical point transition energies (in eV) for 3C-SiC with experimental results. The experimental data are from [41] except where noted otherwise.

| 3C-SiC | Calculation | Measurements |
|--------|-------------|--------------|
| $E_g$  | 2.24        | 2.2[1] 2.4[32] |
| $\Gamma_{15} \rightarrow \Gamma_c$ | 7.23 | 7.4 |
| $L_3 \rightarrow L_1^c$ | 7.02 | 7.5 |
| $X_5 \rightarrow X_1^c$ | 5.39 | 5.8 |
| $X_3^v \rightarrow X_3^c$ | 8.14 | 8.3±0.1 |
| $\Gamma_{15} \rightarrow \Gamma_{15}$ | 8.46 | 9.0±0.2 |
| $L_3 \rightarrow L_3^c$ | 9.27 | 9.4 |

Table 2. The effective masses (in $m_0$) of the n-type carriers at the lowest conduction band of 3C- and 4H-SiC. The theoretical $m_\perp$ of 4H-SiC was calculated as the geometric average of $\sqrt{m_{\Gamma \Gamma} m_{MK}}$.

| 3C-SiC | Calculation | Measurements |
|--------|-------------|--------------|
| $m_{XT}$ | 0.72±0.04 | 0.677 ± 0.015$(m_{nl})[42]$ |
| $m_{XW}$ | 0.22±0.02 | 0.247 ± 0.011$(m_{nl})[42]$ |

| 4H-SiC | Calculation | Measurements |
|--------|-------------|--------------|
| $m_\perp$ | 0.41±0.02 | 0.42[40] |
| $m_{\parallel}(m_{ML})$ | 0.31±0.02 | 0.33 ± 0.01[46] 0.29[40] |
| $m_{\Gamma \Gamma}$ | 0.62±0.03 | 0.58 ± 0.01[46] |
| $m_{MK}$ | 0.27±0.02 | 0.31 ± 0.01[46] |

The effective mass is a measure of the curvature of the calculated bands. The agreement between calculated and measured effective masses indicates an accurate determination of the shape of the bands. Our calculated effective masses of the n-type carriers are listed in table 2. The calculated electron effective mass around the conduction band minimum of 3C-SiC near the X-point is $m_{nl} = 0.72 ± 0.04m_0$ for the $\Gamma$–X direction, and is $m_{nl} = 0.22 ± 0.02m_0$ for the X–W direction. Here, $m_0$ is the free electron mass. The calculated, anisotropic effective masses are in good agreement with the reported experimental data of $m_{nl} = 0.677 ± 0.015m_0$, and $m_{nl} = 0.247 ± 0.011m_0$ [42]. The good agreements of the calculated effective mass and the band-gap with corresponding experimental results indicate that the lowest conduction band in figure 1 is reasonably reliable. Our calculated effective masses are not much different from those of previous LDA calculations, indicating that the extra lowering of the conduction bands, in the absence of the BZW procedure, does not seriously affect the shape of these low-energy conduction bands.

The calculated total and partial density of states (DOS) of 3C-SiC are shown in figure 2 and figure 3. From figures 1, 2 and 3, we can see that the lower valence band ranging from $-15.2$
Figure 2. The total density of states (DOS) of 3C-SiC.

Figure 3. The partial density of states (PDOS) of 3C-SiC.

eV to $-10.0 \text{ eV}$ is dominated by the C(2s) states that are hybridized with the Si(3p) and C(2p) components. The upper valence bands are dominated by the C(2p) states and strongly hybridized with the Si(3p) states. The Si(3d) bands are highly extended and contribute also to the occupied valence bands in the solid-state environment. The conduction band of 3C-SiC has a long tail, ranging from 2.24 eV to about 5 eV, which is attributed to the wide conduction band around the X-point. In figure 2, the extended tail from the conduction band leads to some experimental complications in determining the exact band gap, including the optical absorption edge which can extend to several tenths of an eV. The total DOS curve in figure 2 shows that the ‘practical’ [24] and measurable band gap would be about 2.4 eV.
Figure 4. The calculated total energies of 3C-SiC at different lattice constants in the zinc-blende structure. The minimum total energy is located at a lattice constant of 4.35 Å.

An essential, physical quantity in density functional theory is the ground-state total energy of the system. Recently, we have performed preliminary total-energy calculations for the cubic structures of SiC. The calculated total energies for 3C-SiC at different lattice constants are shown in figure 4. The total energies in figure 4 are computed from the electron charge density using the optimal basis set that is identified by the BZW procedure. The calculated equilibrium lattice constant of 3C-SiC, i.e. the value at the minimum of the total energy curve, is 4.35 Å. This value is in excellent agreement with the experimentally measured lattice constant of 4.348 Å[43]. The calculated bulk modulus of 3C-SiC, from the total energy curve in figure 4, is 2.2 Mbar, which also agrees very well with the experimental value of 2.24 Mbar [44].

3.2. Electronic structure of 4H-SiC

The electronic bands of 4H-SiC along some high symmetry lines are shown in figure 5. The notation of the symmetry points in the Brillouin zone follows the convention used by Koster [39]. The highest occupied state of the valence band is at the Γ-point. The conduction band minimum is at the M-point. There is a second minimum of the conduction band at the M-point, which is only 0.18 eV above the lowest unoccupied state. These results are consistent with the ballistic electron emission microscopy study by Kaczer et al [45] who observed the second minimum of about 0.15 eV above the lowest conduction band minimum in 4H-SiC. The slight difference between these two minima is attributed to both computational and experimental limitations. These limitations include uncertainties introduced in the fit procedure in the analysis of the experimental data and computational uncertainties that include rounding errors. The indirect band-gap from our calculated electron structure of 4H-SiC is 3.11 eV, which is very close to the experimental data of about 3.2–3.3 eV [1, 32].

The calculated effective masses of the n-type carriers around the conduction band minimum of 4H-SiC are also listed in table 2. Our calculated electron effective mass in the plane perpendicular to the c-direction is \( m_{\perp} = 0.41 \pm 0.02 m_0 \), which agrees very well with the
Figure 5. The electronic energy band structure of 4H-SiC along high-symmetry directions, as obtained with the optimal basis set from the BZW procedure.

Figure 6. The total density of states of 4H-SiC.

experimentally measured result of $0.42\ m_0$ [40]. Here, $m_\perp$ is calculated as the geometric average of $\sqrt{m_{\Gamma}m_{MK}}$. The calculated effective masses of the n-type carriers in the direction parallel to the c-direction is $m_{ML} = 0.31 \pm 0.02m_0$, which also agrees well with the experimental results of 0.29–0.33 $m_0$ [40, 46].

The calculated total and partial density of states (DOS) of 4H-SiC are shown in figures 6 and 7. The density of states of 4H-SiC is very similar to that of 3C-SiC. However, the conduction band edge of 4H-SiC does not have the long tail that that of 3C-SiC does.

3.3. Charge transfer in 3C- and 4H-SiC

Both the silicon and carbon atoms have four valence electrons and prefer a four-fold tetrahedral bond arrangement in the formation of compounds. Charge-transfer properties in SiC are consequently not trivial. We calculated the effective charges and charge transfer for 3C- and 4H-SiC, using the ab initio electronic wavefunctions from our computations. Our method
Figure 7. The partial density of states of 4H-SiC.

for calculating the effective charge and charge transfer has been discussed in a previous publication [47].

Our calculated results suggest that the charge transfer in 3C-SiC is very close to that in 4H-SiC, with a difference in the range of computational uncertainty. We found that silicon atoms, in 3C and 4H silicon carbides, give about 1.4 electrons/atom that are gained per carbon atom. The ionic formula for 3C and 4H silicon carbides can be written as Si$^{+1.4}$C$^{-1.4}$. This result, in retrospect, is understandable in the light of more effective shielding of the nucleus in Si as compared with C. The calculational error for the charge transfer was estimated at about ±0.1 electrons.

The charge transfer in 3C- and 4H-silicon carbides occurs mainly in the formation of the Si-C bond. In the formation of the Si-C bond in 3C- and 4H-SiC, the charge transfer is about 0.35 electrons/bond, which is very close to the so-called ‘one third rule’ suggested in the studies of silicon nitride [48, 47].

We also studied the dependence of the charge transfer on the Si-C distance or bond length in 3C-SiC. This dependence is relevant to understanding or simulating the formation of the Si-C bond. We performed ab initio self-consistent calculations for several values of the lattice constant. The calculated results for the charge transfers are listed in table 3. Here, we define the bond length as the distance between Si and C when they are the first nearest neighbours. Table 3 shows that the calculated charge transfer, from Si to C atoms in 3C-SiC, remains nearly constant for a substantially large range of the lattice constant or of the bond length. These results support the practice of assuming that the charge transfer in silicon carbides is a constant, as done in molecular dynamical simulations or in calculations of mechanical properties.
Table 3. The calculated charge transfer, from Si to C atoms in 3C-SiC, at different lattice constants and bond lengths.

| Lattice constant (Å) | Bond length (Å) | Charge transfer (electrons) |
|----------------------|-----------------|----------------------------|
| 4.35                 | 1.884           | 1.4                        |
| 4.50                 | 1.949           | 1.4                        |
| 5.00                 | 2.165           | 1.5                        |
| 6.00                 | 2.598           | 1.4                        |
| 7.00                 | 3.031           | 1.4                        |
| 8.00                 | 3.464           | 1.2                        |
| 9.00                 | 3.897           | 1.1                        |

4. Conclusion

We have calculated the electronic structures of 3C- and 4H-SiC, using the \textit{ab initio} LCAO method and the newly developed BZW procedure. Our calculated valence band structures of 3C- and 4H-SiC agree with previous results from first-principle calculations. Our calculated band-gaps, effective masses of n-type carriers, and critical point transition energies agree well with experimental results. Our preliminary total energy calculations for 3C-SiC led to an equilibrium lattice constant of \( a = 4.35 \) Å, which is in an excellent agreement with experiment. Our calculated results suggest that the charge transfer in 3C-SiC is very close to that in 4H-SiC. The silicon atoms, in 3C and 4H silicon carbides, give about 1.4 electrons/atom to the carbon atoms. For a substantially large range of the bond length, the calculated charge transfer from Si to C atoms remains nearly constant in 3C-SiC.

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