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Theoretical study on the band structure and optical properties of 4H-SiC*

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We have studied the band structure and optical properties of 4H-SiC by using a full potential linearized augmented plane waves (FPLAPW) method. The density of states (DOS) and band structure are presented. The imaginary part of the dielectric function has been obtained directly from the band structure calculation. With band gap correction, the real part of the dielectric function has been derived from the imaginary part by the Kramers–Kronig (KK) dispersion relationship. The values of reflectivity for normal incidence as a function of photon energy have also been calculated. We found the theoretical results are in good agreement with the experimental data.

Keywords: 4H-SiC, FPLAPW, band structure, optical property
PACC: 7115A, 7865P

1. Introduction

SiC has attracted much interest because of its significant technological importance for high temperature, high power, high critical breakdown field and high frequency applications in microelectronic and photoelectronic devices.[1] It is very important to know the optical properties of SiC due to their contributions to the photoelectronic device design. However, theoretical studies on the optical properties of SiC have been scarce up to now. We have investigated the surface structure of SiC by the full potential linearized augmented plane waves (FPLAPW) method before.[2] In this paper, we report a first-principles calculation of the band structure and optical properties of 4H-SiC by using the FPLAPW method based on density function theory and compare the theoretical values with available experimental results.

2. Calculation method

The basic principle of the FPLAPW method can be found in Ref.[3]. The Kohn–Sham equations and energy functionals are evaluated self-consistently using the FPLAPW method. We use parameters $R_{\rm MT}K_{\rm max}$=8 to determine the matrix size (convergence), where $K_{\rm max}$ is the plane wave cut-off and $R_{\rm MT}$ is the smallest atomic sphere radii. In the atomic regions, the basis set consists of spherical harmonics with angular quantum number l $\leq$10 and a nonspherical contribution with $l \leq 4$. We choose the muffin-tin (MT) radii of Si and C to be 1.8 and 1.7 a.u. respectively. As we know, in a full potential calculation the choice of MT radii should not affect the final results provided that the calculations are well converged. The lattice parameters are taken from the experimental data. We choose the exchange-correlation potential parametrized by Perdew *et al*[4] which is derived by using the generalized gradient approximation (GGA). The Si 1s and 2s states as well as C 1s state are considered as core states. The self-consistent iterations are considered to be converged when the total energy of the system are stable within 10^{-3} mRy. The integrals over the Brillouin zone are performed using the Monkhorst–Pack[5] special k-points approach. Since the calculations of optical properties require more dense k-space matrix, we use 7000 k-points for the calculations of dielectric function.

The dielectric function of a solid is usually described in terms of a complex parameter as $\varepsilon(\omega)$ =

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$\varepsilon_1(\omega)+i\varepsilon_2(\omega)$, in which the imaginary part $\varepsilon_2(\omega)$ can be obtained directly from the band structure calculation. While the real part $\varepsilon_1(\omega)$ can be derived from the imaginary part $\varepsilon_2(\omega)$ by using the Kramers–Kronig (KK) dispersion relationship. The longitudinal and transverse dielectric functions are calculated separately, where the longitudinal direction is along the c-axis and the transverse direction is in the plane perpendicular to the c-axis. Furthermore, the reflectivity coefficient R can also be derived from the relationship among the optical constants. In order to correct the error in the band gap due to local density approximation (LDA), we apply a constant potential to shift the conduct band states rigidly in order to match the calculated band gaps with the experimental data.

3. Results and discussion

Figure 1(a) shows the partial DOS for Si atom and C atom in 4H-SiC. Solid, dashed and dotted lines represent s-, p-, d-like states respectively. The energy scale takes the top of valence band (VB) as reference. There are two sub-bands in the VB. The lower one is composed of Si 3s, Si 3p and C 2s. While the higher one is composed of Si 3s, Si 3p, Si 3d, C 2s and C 2p, where Si 3s and C 2p are mainly in the low energy range, and Si 2p and C 2p are mainly in the high energy range.

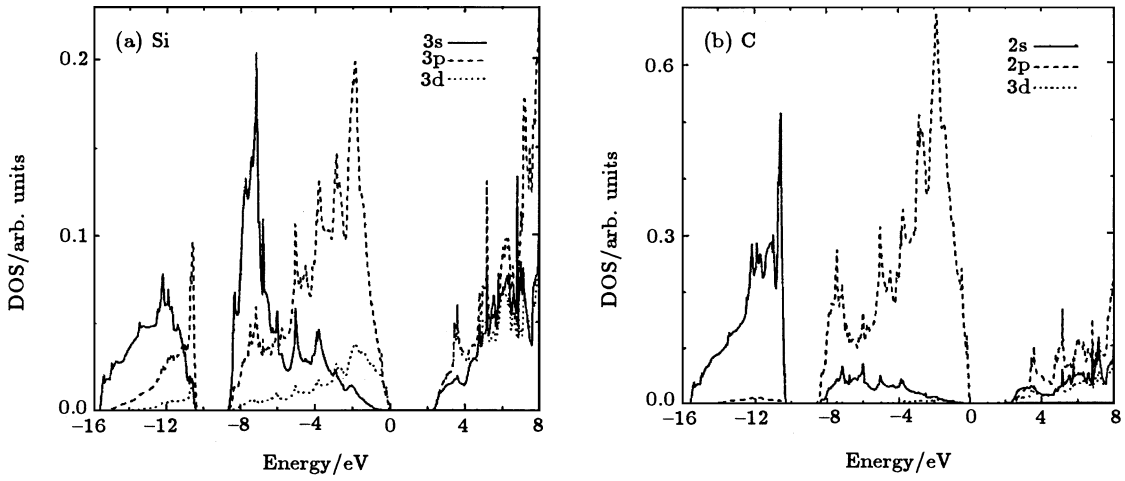


Fig.1. The partial DOS for Si (a) and C (b) atoms in 4H-SiC.

The calculated band structure of the intrinsic 4H-SiC crystal is plotted in Fig.2. The general characteristic is similar to that of 2H-SiC,[6] but the width of the Brillouin zone along the z direction decreases by about 50%. The calculated VB maximum is at Γ point. The conduction band (CB) minimum is located at M point. The calculated band gap is 2.25eV, which is about 31.6% less than the experimental result. It is well known that a deficiency of the local density theory is that the calculated value of the fundamental energy gap is smaller than the experimental one. However, it is reasonable to believe that the band structure and optical properties can accurately be described by LDA. Furthermore, the second lowest conduction-band minimum is located at the M point, separated by only 120meV from the lowest minimum. The energy difference is close to the energy of the optical phonon energies of 0.0104–0.121eV[7] and the second band will therefore influence the transport properties at high temperature of high applied electric field.

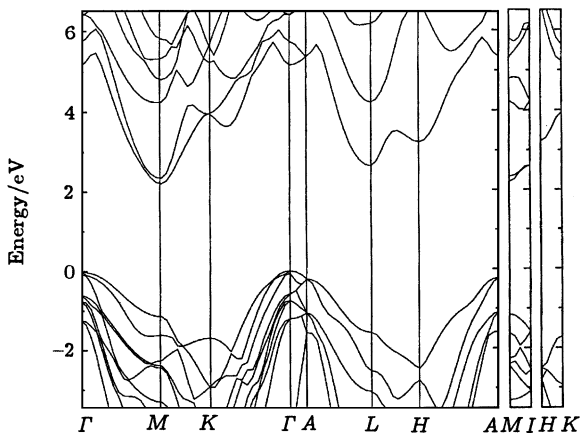


Fig.2. The band structure of 4H-SiC.

From the band structure and the partial DOS, we can calculate the imaginary part $\varepsilon_2(\omega)$ of the di-

electric function as a function of photon energy along the transverse and the longitudinal directions respectively, as shown in Fig.3. Here we have taken into consideration the band gap correction ΔE_g=1.04eV, which shifts the calculated $\varepsilon_2(\omega)$ upward. After band gap correction, the real part of the dielectric function $\varepsilon_1(\omega)$ can be derived from $\varepsilon_2(\omega)$ according to the KK dispersion relationship and is shown in Fig.4. In Figs.3 and 4, the solid lines are the calculated results, while the dotted lines indicate the recent experimental results measured by Lindquist and Jarrendahl[8] by using ultraviolet spectroscopic ellipsometry.

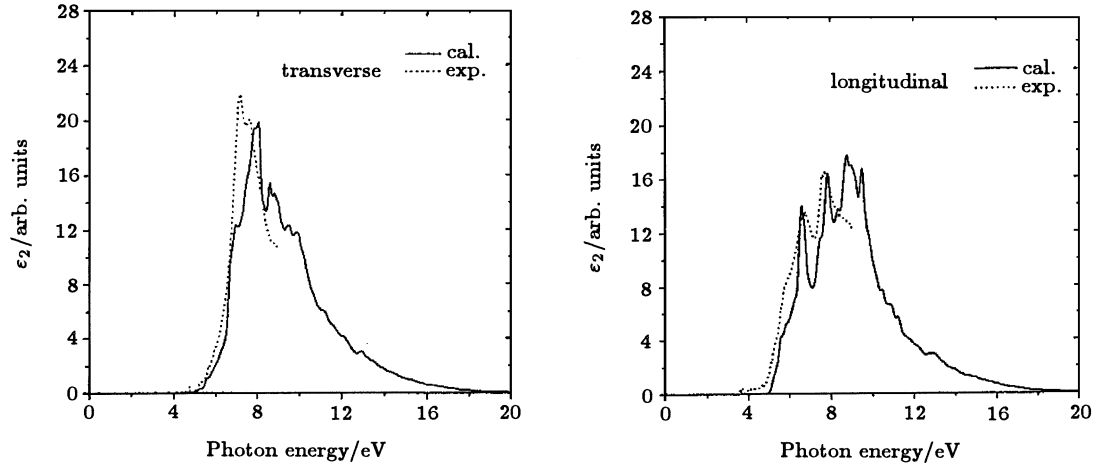


Fig.3. The transverse and the longitudinal components of the imaginary part ε_2 of the dielectric function as functions of photon energy. Solid and dotted lines represent the calculated and experimental results respectively.

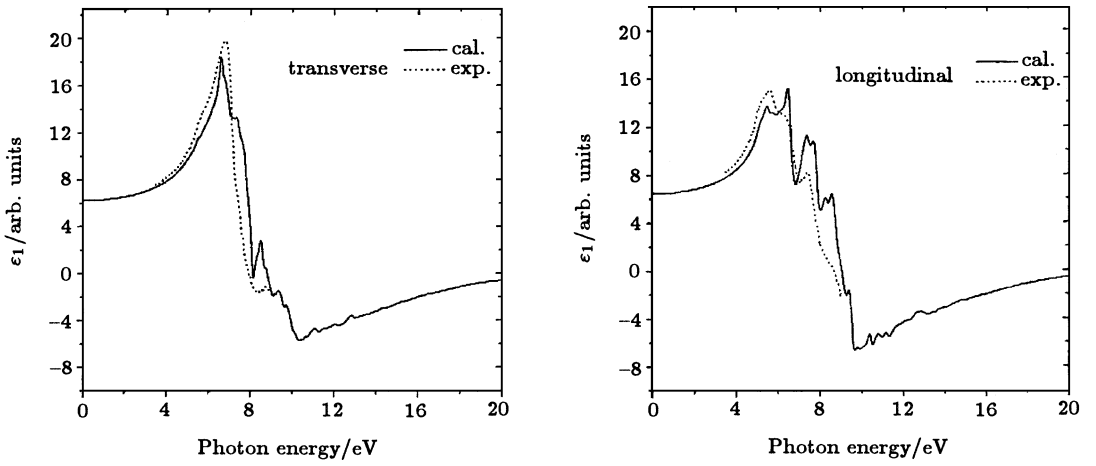


Fig.4. The transverse and the longitudinal components of the real part ε_1 of the dielectric function as functions of photon energy. Solid and dotted lines represent the calculated and experimental results respectively.

The optical absorption and transition can be identified by the imaginary part $\varepsilon_2(\omega)$ of the dielectric function as a function of photon energy. Compared with 2H-SiC,[6] the analysis on 4H-SiC in terms of band-to-band transition is much more complicated because of the decrease of the Brillouin zone width along the z direction and a large number of bands being folded into the small Brillouin zone. There are a number of critical points exhibited in the calculated dielectric function. The absorption starts at about 4.36eV, which is related to the direct transitions from the VB top to the CB minimum at M point. In the transverse direction, the critical point at 7.03eV may come from the direct transition between the second lowest CB minimum and the highest VB top at the H point. In the longitudinal direction, there are two critical points located at 5.56eV and 6.62eV respectively. The former one is probably from the transition along

the ML line, which is consistent with the calculated result of Adolph *et al.*[9] The latter may come from the direct transition between the second lowest CB minimum and the VB top at L point, which is similar to Ahuja *et al*'s calculated result.[10] The critical point at 7.8eV exists in both directions, which is probably related to the direct transition at the K point. The experimental results of Lindquist *et al*[8] reveal a group of critical points at 7.12 and 7.62eV in the transverse direction, which correspond respectively to the values of 7.03 and 7.8eV in our calculation. They have also obtained a group of critical points at 5.6, 6.63 and 7.62eV experimentally in the longitudinal direction, which are also consistent with the values of 5.56, 6.62 and 7.8eV in our calculation results. It shows that the calculated results for the critical point positions are in good agreement with the experimental data. Furthermore, we have also calculated the high-frequency dielectric constant $\varepsilon_1(\infty)$. The values of it in the transverse direction and the longitudinal directions are 6.25 and 6.44 respectively, which are slightly less than the experimental values of 6.52 and 6.70 measured by Coyke.[11] Obviously, the calculated values of $\varepsilon_1(\infty)$ are in good agreement with the experimental results.

From the imaginary and real parts of the dielectric function, we can calculate the other important optical constants. In Fig.5, we present the reflectivity curves as a function of photon energy along transverse direction for normal incidence. The solid line shows calculated results, while the dotted line shows the experimental results of Lambrecht *et al.*[12] In general, the calculated results are in fairly good agreement with the experimental ones. Both have similar critical point structure. The values of theoretical reflectivity are smaller than the experimental values at energies less than 7.8eV. But they are much higher than the experimental ones at energies beyond 8.5eV. It is probably attributed to the enhancement of scattered reflection due to the surface roughness of the sample in the range of high photon energy, which affects the experimental results and produced the large difference between the theoretical and experimental results.

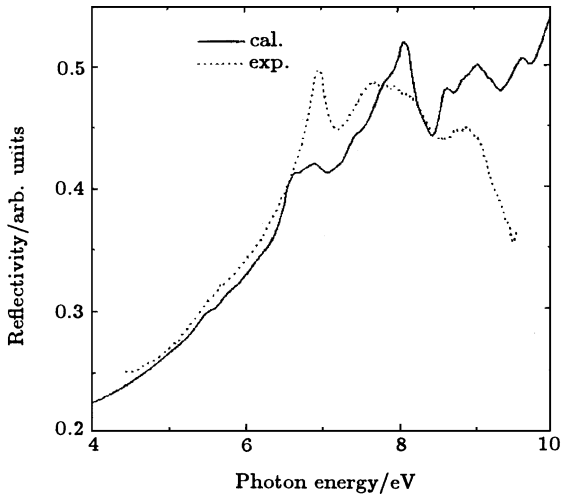


Fig.5. The reflectivity curves of 4H-SiC as a function of photon energy along the transverse direction for normal incidence. Solid and dotted lines represent the data from calculated and experimental results respectively.

4. Conclusion

In conclusion, we have carried out calculations for the band structure and optical properties of 4H-SiC. The calculated dielectric function values are in good agreement with the experimental results. The critical point structure of the dielectric function is investigated and analysed to identify the optical transition. The calculated reflectivity has the similar structure to the experimental results.

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