

First-principles calculation of free carrier absorption in 4H-SiC

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Abstract—Free carrier absorption (FCA) spectra for 4H-SiC are calculated using a first-principles framework based on density functional theory. The spectra are obtained for two different polarization directions: $E \parallel c$ and $E \perp c$. For n -type 4H-SiC, our calculated spectra show two strong absorption peaks, which are in good agreement with the experimental results. For the p -type 4H-SiC, our calculations predict three absorption peaks in the infrared spectral region. Our results demonstrate the possibility of a SiC-based optical attenuator that exploits FCA as the loss mechanism with carrier density as the control parameter.

Index Terms—4H-SiC, free carrier absorption, density functional theory

I. INTRODUCTION

Free carrier absorption (FCA) is an intraband absorption mechanism in which free electrons (holes) in the conduction (valence) band absorb photon energy, resulting in optical attenuation. FCA becomes stronger in heavily doped semiconductor materials and makes significant contributions to the total absorption. In indirect-bandgap semiconductors such as 4H silicon carbide (SiC), momentum conservation requires the simultaneous participation of a phonon or an ionized impurity, making FCA an intrinsically phonon- or impurity-assisted indirect process. Consequently, the FCA cross section depends sensitively on the dominant scattering mechanism. A quantitative description of FCA, therefore, requires a full account of the electronic band structure, the phonon dispersion, and the electron-phonon coupling strength throughout the Brillouin zone.

4H-SiC is a promising wide-bandgap material for integrated photonics. Its high thermal conductivity ($4.9 \times 10^2 \text{ W m}^{-1} \text{ K}^{-1}$) [1] enables efficient heat dissipation from FCA and supports high-power attenuation without thermal runaway. Its high critical electric field (2.8 MV cm^{-1}) [1] allows operation at high voltages without breakdown. Thus, it is well-suited for high-power and high-temperature applications.

Recently, a general first-principles framework based on density functional theory (DFT) that accounts for the indirect processes was proposed and successfully applied to both n -type and p -type silicon [2]. In this work, we applied the methodology to compute the FCA spectra in both n -type and p -type 4H-SiC. The results are compared with recent pump-probe measurements of optical resonance peaks in n -

type 4H-SiC [3]. Our results identify the dominant phonon-assisted scattering channels governing FCA across the relevant spectral range and establish quantitative, carrier-concentration-dependent absorption coefficients directly applicable to photonic device modeling.

II. METHOD

The electronic structure of 4H-SiC was obtained using the Quantum Espresso (QE) package [4], [5]. The SG15 optimized norm-conserving Vanderbilt (ONCV) pseudopotential [6], [7] has been used to express the core-valence interactions. An $8 \times 8 \times 4$ Γ -centered grid of $\mathbf{k}$ -points in the first Brillouin zone with a plane wave energy cutoff of 120 Ry is sufficient to reach convergence of the total energy, with an error within 0.1 mRy per atom. The Heyd-Scuseria-Ernzerhof (HSE) hybrid functional [8], [9] with 25% of exact exchange gives 3.17 eV indirect energy gap. The phonon dispersion and electron-phonon coupling matrix elements were obtained using density functional perturbation theory (DFPT) [10], [11] implemented in QE with the PBE functional [12] using an $8 \times 8 \times 4$ grid of phonon $\mathbf{q}$ -vectors. FCA was calculated using EPW code [2], [13]–[16], where four different contributions to FCA were considered within a general first-principles framework: (i) direct, (ii) phonon-assisted, (iii) charged-impurity-assisted, and (iv) the semiclassical resistive Drude processes. The absorption coefficients were obtained from the imaginary part of the dielectric function, assuming a constant refractive index of 2.6 [1] throughout the spectral range of interest. The total impurity density (N_{imp}) dependent electron and hole mobilities, which are necessary for the Drude process calculations, at $T = 300 \text{ K}$ were obtained from empirical fits to experimental data:

$$\mu_n(300, N_{\text{imp}}) = \frac{977}{1 + \left(\frac{N_{\text{imp}}}{1.17 \times 10^{17}}\right)^{0.49}}, \quad (1)$$

for electron mobility [17] and

$$\mu_p(300, N_{\text{imp}}) = 37.6 + \frac{68.4}{1 + \left(\frac{N_{\text{imp}}}{2.97 \times 10^{18}}\right)^{0.356}}, \quad (2)$$

for hole mobility [18], where mobilities are expressed in $\text{cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ and N_{imp} in cm^{-3} .

III. RESULTS

Figure 1 (a) shows the electronic band structure of 4H-SiC. The band structures near the conduction band minimum (CBM) at M and the valence band maximum (VBM) at Γ are denoted by red and green boxes, respectively. The region near the CBM is shown in Fig. 1 (b). The six lowest bands at M point are labeled from c_0 to c_5 . The transition from c_0 to c_2 is shown as A1 with a blue solid line, whereas the transition from c_0 to c_3 is shown as B1 with a red solid line. The region near the VBM is shown in Fig. 1 (c). The five highest bands at the Γ point are labeled from v_0 to v_4 . The transitions from v_0 to v_2 (C1) and v_0 to v_3 (C2) are shown in a red solid line, whereas the transition from v_0 to v_4 (D1) is shown in a solid blue line.

Figure 2 (a) shows the experimental measurement of the FCA for n -type 4H-SiC ($n = 4 \times 10^{17} \text{ cm}^{-3}$ electron concentration) performed by Grivickas *et al.* [3]. There are two strong peaks labeled as A1 and B1. The peak A1 was obtained by the $E \parallel c$ polarization and is located at 2.08 eV corresponding to the A1 transition between bands c_0 and c_2 shown in Fig. 1 (b). The peak B1 was obtained by the $E \perp c$ polarization and is located at 2.66 eV corresponding to the transition between bands c_0 and c_3 also shown in Fig. 1 (b). Figure 2 (b) shows our calculated results of the absorption coefficients, which were obtained with $E \parallel c$ and $E \perp c$ polarizations. The electron concentration is assumed to be $1 \times 10^{19} \text{ cm}^{-3}$. All three contributions (phonon-assisted, charged-impurity-assisted, and direct processes), except for the resistive contribution, which is nearly zero in this energy range, are plotted in dashed, dotted, and dashed-dotted lines, respectively. The phonon-assisted process dominates the FCA spectra across the entire energy range. The peak A1 is located at 2.08 eV with $E \parallel c$ polarization, and the other peak B1 is located at 2.60 eV with $E \perp c$ polarization. These peaks correspond to the transitions from the bottom of the conduction band (c_0) to the bands c_2 and c_3 , respectively [see Fig. 1 (b)]. The absorption occurs in the visible spectral window. Our calculated results agree well with the experimental results shown in Fig. 2 (a). Figure 2 (c) shows our calculated results for p -type 4H-SiC. The hole concentration is assumed to be $1 \times 10^{19} \text{ cm}^{-3}$. The phonon-assisted process denoted by the dashed line makes the largest contribution, as in the n -type case. There are three peaks at 0.63 eV (C1), 0.79 eV (C2), and 1.29 eV (D1). These peaks correspond to the transitions from the top of the valence band (v_0) to the bands v_2 , v_3 , and v_4 , respectively [see Fig. 1 (b)]. The peaks C1 and C2 are prominent with the $E \perp c$ polarization, while the peak D1 is observed only with the $E \parallel c$ polarization. The absorption occurs in the infrared spectral window.

In Fig. 3, the dependence of the FCA spectra on carrier concentration is shown. For both n -type [Fig. 3 (a)] and p -type [Fig. 3 (b)], the absorption coefficient increases monotonically with carrier concentration across the entire spectral range while the spectral peak positions remain unchanged. Although carrier concentrations exceeding $1 \times 10^{19} \text{ cm}^{-3}$

are experimentally challenging, particularly for p -type 4H-SiC, the calculations show that higher doping levels yield substantially larger absorption coefficients, enabling effective optical attenuation that is continuously tunable via the free-carrier density.

IV. CONCLUSION

We have shown first-principles calculations of free carrier absorption spectra in both n -type and p -type 4H-SiC, employing the ab initio framework of Zhang *et al.* [2] For n -type 4H-SiC, the computed spectra exhibit two strong absorption peaks at 2.08 eV (A1, $E \parallel c$) and 2.60 eV (B1, $E \perp c$), in good agreement with the pump-probe experimental data of Grivickas *et al.* [3], validating the theoretical framework for this material. For p -type 4H-SiC, three absorption peaks are predicted in the infrared: C1 (0.63 eV) and C2 (0.79 eV) under $E \perp c$ polarization, and D1 (1.29 eV) under $E \parallel c$ polarization. In both doping types, the phonon-assisted process constitutes the dominant FCA mechanism, confirming the central role of electron-phonon coupling in determining the intraband optical response of 4H-SiC. The FCA absorption coefficient scales monotonically with carrier concentration for both doping types, demonstrating that the free-carrier density can serve as an effective control parameter for optical attenuation. The pronounced polarization dependence of FCA with spectrally distinct peak positions for $E \parallel c$ and $E \perp c$ further offers a route to polarization-selective attenuation in integrated photonic circuits.

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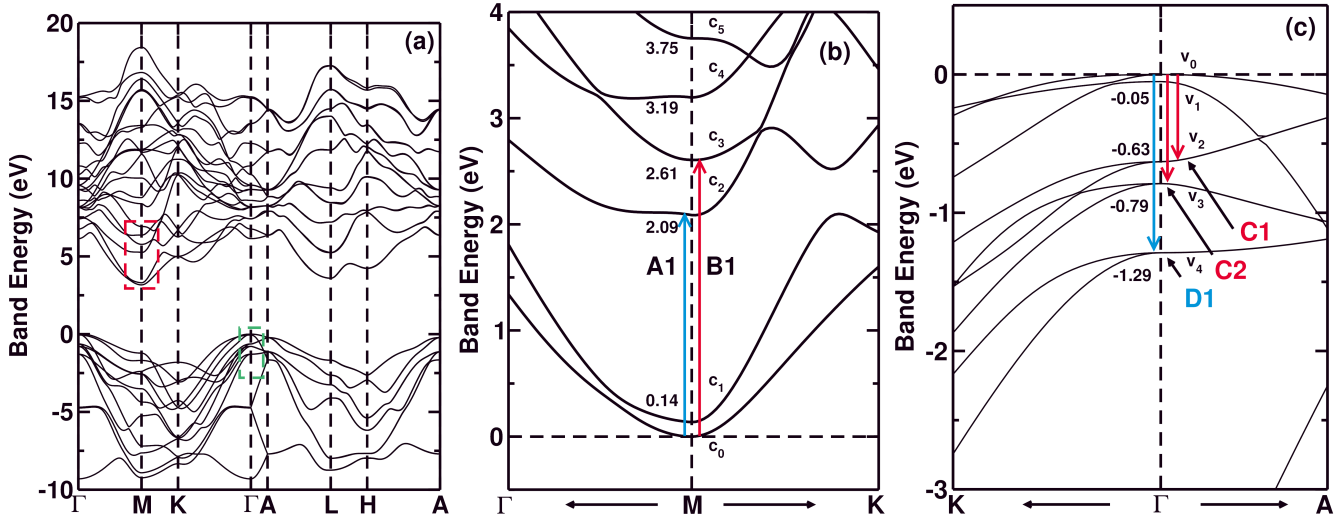


Fig. 1. (a) Electronic band structure of 4H-SiC. (b) Around the conduction band minimum at M point, denoted by the red box in (a), with six bands from c_0 to c_5 . The transition between the bands c_0 and c_2 is denoted as A1, (blue solid line) and the transition between the bands c_0 and c_3 is denoted as B1 (red solid line). (c) Around the valence band maximum at Γ point, denoted by the green box in (a), with five bands from v_0 to v_4 . The transition between the bands v_0 and v_2 is denoted as C1 (red solid line), the transition between the bands v_0 and v_3 is denoted as C2 (red solid line), and the transition between the bands v_0 and v_4 is denoted as D1 (blue solid line).

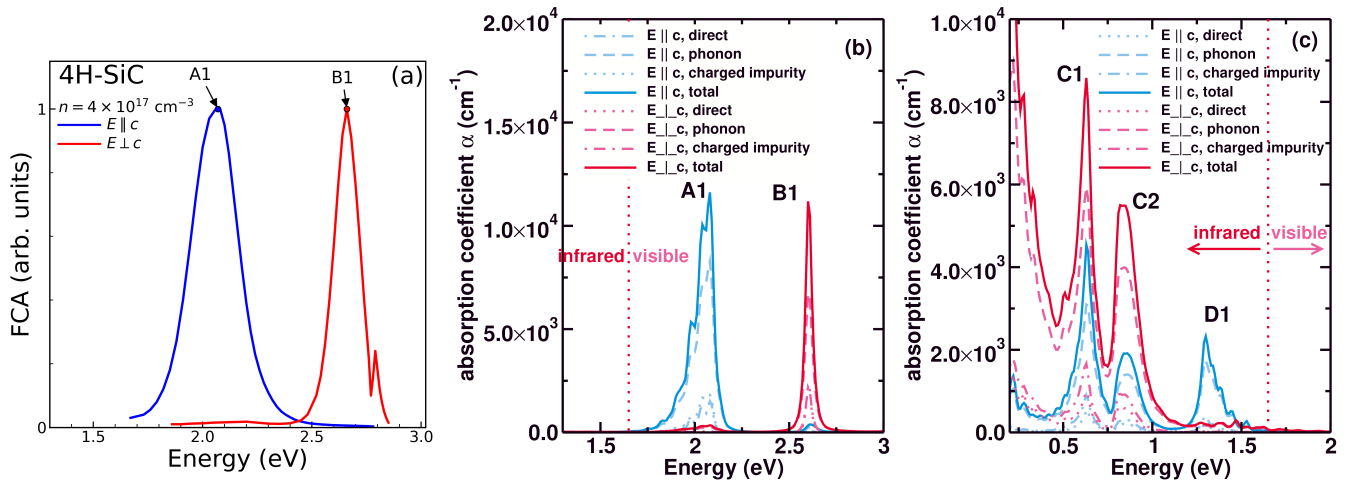


Fig. 2. (a) Free carrier absorption spectra for n -type 4H-SiC, measured by Grivickas *et al.* [3] Two different polarizations are considered: $E \parallel c$ in solid blue line with the peak A1 and $E \perp c$ in solid red line with the peak B1. (b) Calculated free carrier absorption spectra for n -type 4H-SiC. Our result agrees well with the experimental result shown in (a). The contribution from the phonon-assisted process (dashed lines) is dominant. The peaks A1 and B1 correspond to the transitions from c_0 to c_2 and from c_0 to c_3 , respectively [see Fig. 1 (b)] (c) Calculated free carrier absorption spectra for p -type 4H-SiC. The contribution from the phonon-assisted process (dashed lines) is dominant. The peaks C1, C2, and D1 correspond to the transitions from v_0 to v_2 , from v_0 to v_3 , and from v_0 to v_4 , respectively.

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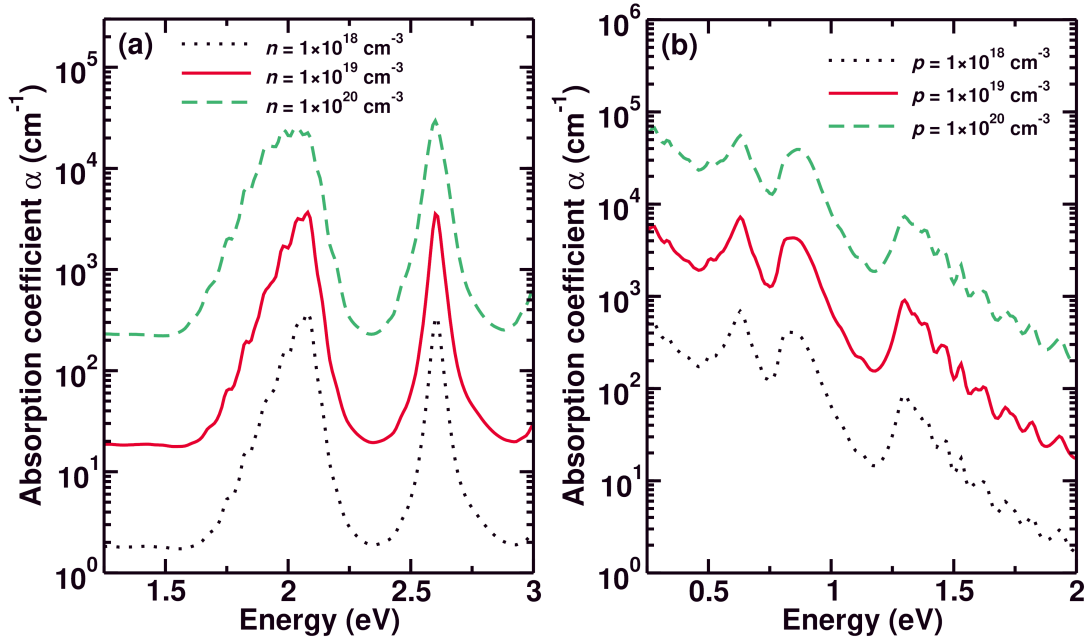


Fig. 3. Calculated free carrier absorption spectra for different carrier concentrations. (a) n -type with 1×10^{18} , 1×10^{19} , and $1 \times 10^{20} \text{ cm}^{-3}$ electron concentrations. (b) p -type with 1×10^{18} , 1×10^{19} , and $1 \times 10^{20} \text{ cm}^{-3}$ hole concentrations.

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