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DFT Study of Armchair Silicon Carbide Nanoribbons (w=3)

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Abstract

The optical spectra of armchair silicon carbide nanoribbons (ASiCNRs) with edges passivated by hydrogen were calculated exploiting density functional theory (DFT). It was found that the dielectric function of the simulated nanoribbon has anisotropic behavior due to the asymmetric crystal lattice. Compared to isotropic behavior, anisotropic means different behavior in all directions. The first peak of the imaginary part of the dielectric function (2.57 eV) suggests that the first optical band-gap of ASiCNRs is 2.57 eV. Besides, the z component of the static refractive index of ASiCNRs is 1.34. Our results show that the first optical absorption's peak for the z polarization happens at 2.57 eV, which is in agreement with the imaginary part of the dielectric function. The first and second peaks of the optical extinction are located at 2.57 eV and 3.42 eV as well.

1. Introduction

Silicon carbide (SiC) is a promising material for comprehending nonlinear and quantum photonics sciences [1-4]. Silicon Carbide optics are becoming popular in high-energy laser (HEL) designs [5]. SiC is an outstanding material in thermally variable environments and HEL applications due to its excellent thermal stability, high specific stiffness with a low coefficient of thermal expansion (CTE), and resonant frequency advantages over materials like Zerodur (https://www.techbriefs.com/component/content/article/tb/supplements/pit/features/articles/40201). Zerodur is a zero expansion glass-ceramic material [6-8]. SiC is quickly emerging as a leading platform for the implementation of nonlinear and quantum photonics [9]. SiC is a unique composite material developed for applications in semiconductor lithography and other industries. This advanced material has the highest combination of mechanical and thermal stability and can be optically polished, making it perfect for laser targeting and communications applications. SiC is also exploited in commercial applications such as reflective imaging systems, semiconductor wafer handling, and lightweight scan mirrors (https://apertureos.com/products/sic-optics/).

Nanoscience and nanotechnology can be utilized across all science fields, such as physics, chemistry, materials science, biology, and engineering. Nowadays, researchers are finding different methods to deliberately make the bulk materials at the nanoscale to take advantage of their improved properties such as lighter weight, higher strength, greater chemical reactivity than their larger-scale counterparts, and increased control of light spectrum (https://www.nano.gov/nanotech-101/what/definition). In this work, we study the dielectric function, static refractive index, optical absorption, and optical extinction of armchair SiCNRs (ASiCNRs) (w=3) with edges passivated by hydrogen exploiting density functional theory (DFT). Then, we compare the results with the available data to study the effect of width (w) on the optical spectra.

2. Materials and Methods

2.1 *Simulation method*

The ongoing calculations are conducted within the DFT framework as performed in SIESTA software [10]. The generalized gradient approximation (GGA) with the Perdew-Burke-Enzerhof (PBE) method has been used to simulate exchange-correlation (XC) functional [11]. The energy cut-off is set to 150 Ry. An orthorhombic unit cell was selected as a SiCNR (w=3) crystal lattice (Figure 1). The silicon, hydrogen, and carbon elements are represented by yellow, white, and gray spheres, respectively. After the optimization of SiCNR (w=3), the real and imaginary parts of the dielectric function, optical absorption, refractive index, and optical extinction are calculated via the Monkhorst-Pack 1×1×120 k-point mesh for Brillouin zone sampling.

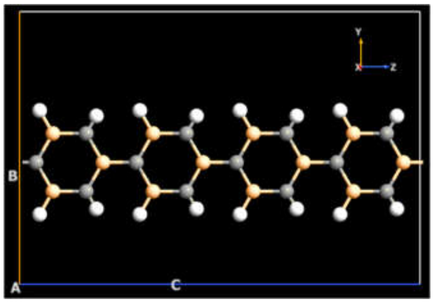

Figure 1. ASiC nanoribbon (w=3) crystal lattice with edges passivated by hydrogen

3. Results and Discussion

3.1 *Optical spectra*

The real part of the dielectric function ($\mathrm{Re}\varepsilon_{\sigma\rho}(\omega)$) can be defined via the Kramers–Kronig equation:

$$\mathrm{Re}\varepsilon_{\sigma\rho}(\omega) = \delta_{\sigma\rho} + \frac{2}{\pi} \mathrm{P} \int_0^\infty \frac{\omega' \mathrm{Im}\varepsilon_{\sigma\rho}(\omega')}{\omega'^2 - \omega^2} d\omega' \qquad (1)$$

where σ and ρ are the directional components. The imaginary part of the dielectric function, $\mathrm{Im}\varepsilon_{\alpha\beta}$, is a function of the electronic charge magnitude (e), electronic mass (m), occupied valence (v_k) , and empty conduction states (c_k) [12]:

$$\mathrm{Im}\varepsilon_{\sigma\rho}^{(inter)}(\omega) = \frac{\hbar^2 e^2}{\pi \mathrm{m}^2 \omega^2} \sum_{c} \int dk \langle c_k | P^{\sigma} | v_k \rangle \langle v_k | P^{\rho} | c_k \rangle \times \delta(\varepsilon_{ck} - \varepsilon_{vk} - \omega) \tag{2}$$

Figure 2 shows the real and imaginary parts of the dielectric function of ASiCNRs. The graphs confirm that the dielectric function of the simulated nanoribbon has anisotropic behavior due to the asymmetric crystal lattice. The first peak of the imaginary part of the dielectric function (2.57 eV) suggests that the first optical band-gap of ASiCNRs is 2.57 eV.

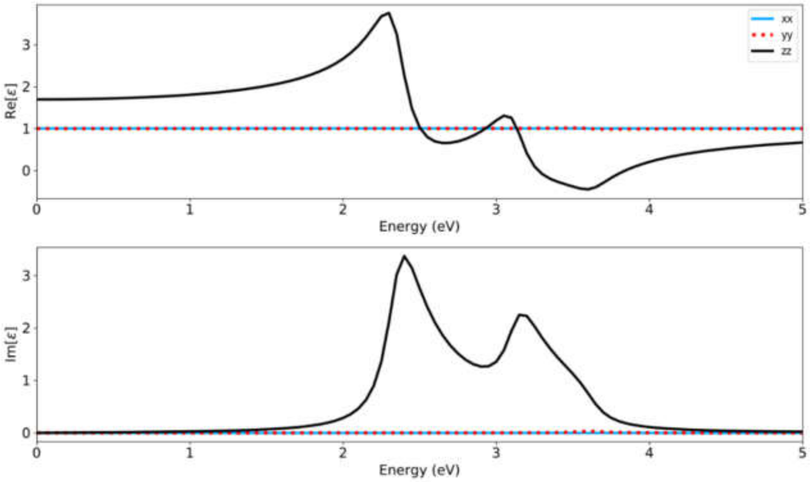

Figure 2. Real and imaginary parts of the dielectric function of ASiCNRs

The optical refractive index has been obtained using the following formula [13]:

$$n(\omega) = \sqrt{\varepsilon_1(\omega)} \tag{3}$$

The z component of the static refractive index of ASiCNRs (w=3) is 1.34. The refractive index of ASiCNRs has not been reported yet. The previous study suggests that the static refractive index of zigzag silicon carbide nanoribbons ZSiCNRs (w=14, 16, 18, 20) is 1.10 and 1.05. Based on the data, the nanoribbons with smaller widths have a larger refractive index. This statement is in agreement with our result (the width of ASiCNRs (w=3) is smaller than that of ZSiCNRs (w=14, 16, 18, 20) [14].

The refractive index graph is represented in Figure 3.

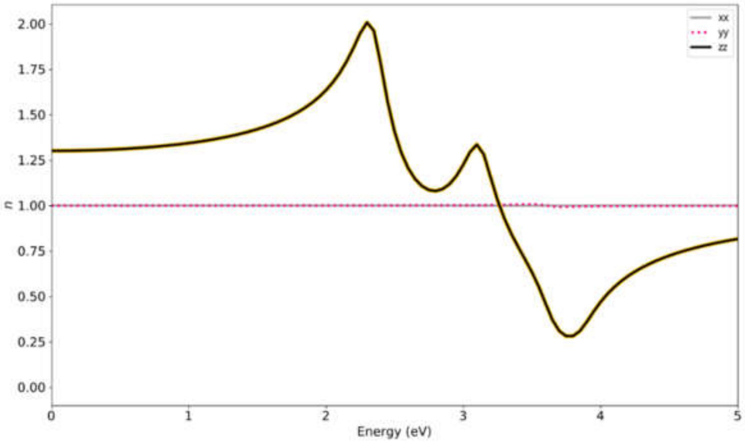

Figure 3. Refractive index of the dielectric function of ASiCNRs

Studying the optical absorption has proved to be a useful method to understand the optical behavior of the materials. In particular, the optical transitions in the band-gap of the material can be studied by calculating the optical absorption spectra [15, 16]. Figure 3 shows the optical absorption of ASiCNRs. From the graph, it is clear that the first optical absorption's peak for the z polarization happens at 2.57 eV, which is in agreement with the imaginary part of the dielectric function. In comparison, for x and z polarizations of ZSiCNRs (w=14, 16, 18, 20), the first optical absorptions occur in the energy range ~0.2 eV and ~1.2 eV, respectively [14].

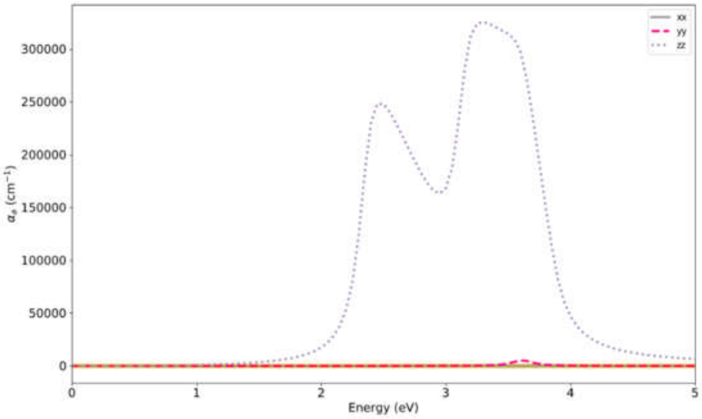

Figure 3. Optical absorption of ASiCNRs

The refraction of light, R(ω), as a function of n (refractive index) and k (extinction coefficient), is the bending of a wave when light passes in a normal incidence case from one medium to another with different speeds [15]:

$$R_{ii}(\omega) = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2} \tag{4}$$

where n and k are the real and the imaginary part of the complex refractive index, respectively[15]:

$$n_{ii}(\omega) = \frac{|\epsilon_{ii}\ (\omega)| + Re\ \epsilon_{ii}\ (\omega)}{2} \tag{5}$$

$$k_{ii}(\omega) = \frac{|\epsilon_{ii}\ (\omega)| - Re\ \epsilon_{ii}\ (\omega)}{2} \tag{6}$$

The optical extinction of armchair silicon carbide nanoribbons (w=3) is shown in Figure 4. The data shows that the first and second peaks of the optical extinction are located at 2.57 eV and 3.42 eV.

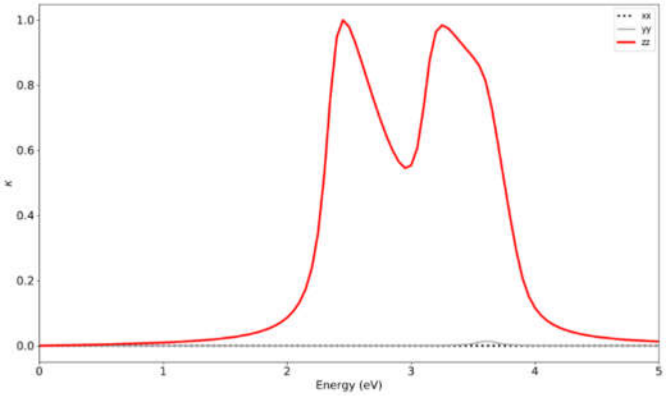

Figure 4. Optical extinction of ASiCNRs

4. Conclusions

The well-known density functional non-equilibrium framework has been used to calculate the optical spectra of armchair silicon carbide nanoribbon (w=3). Our results suggest that the dielectric function of ASiCNR has anisotropic behavior due to the asymmetric crystal structure. Moreover, the first peak of the imaginary part of the dielectric function (2.57 eV) suggests that the first optical band-gap of ASiCNRs is 2.57 eV. In particular, the optical transitions in the band-gap of the material can be studied by calculating the optical absorption spectra. The output indicates that the first optical absorption's peak for the z polarization happens at 2.57 eV, which is in agreement with the imaginary part of the dielectric function.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding this article.

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