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Phonon Spectra of Monolayer Silicon Carbide

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Abstract

Silicon carbide monolayer is a promising material in the semiconductor industry. The silicon and carbon elements in the two-dimensional silicon carbide are arranged in a two-dimensional hexagonal lattice. The quantum of the crystal lattice vibrations, namely phonons, dominate mainly the physical characteristic of the crystals as a result of electron mobility. It is clear that the number of phonons is zero, from 85 meV to 117 meV. In addition, the silicon carbide monolayer sees its phonon density of states (PDOS) maximum at 140 meV, confirming that there are more allowed phonon energy levels at this point of energy. There are four peaks from 0 eV to 85 eV, indicating optical phonons and zone boundary (ZB) phonons. For the low-range energy, all electronic sub-bands correlate acoustic phonons, where the transverse acoustic phonons have lower energy than the longitudinal acoustic modes.

1. Introduction

Silicon carbide is composed of carbon and silicon atoms with strong bonds in the tetrahedral crystal lattice, which results in very hard and strong material. Silicon carbide (SiC) is a chemical compound of carbon and silicon with good mechanical properties, including thermal shock resistance and high temperature strength. Silicon carbide can be produced via two methods. The silicon reacts with the carbon forming SiC. It can be produced using a high temperature electro-chemical reaction of carbon and sand [1]. Today, the material has been developed into a high quality technical grade ceramic with very good mechanical properties. It is used in refractories, abrasives, ceramics, and high-performance applications [2]. The structural and wear applications of silicon carbide are constantly developing. The electrical conduction of the material has led to its utilization in resistance heating elements for electric furnaces, and as a key component in temperature variable resistors and in voltage variable resistors. It has found application in heating elements and refractory linings for industrial furnaces, in semiconducting substrates for light-emitting diodes, and in wear-resistant parts for pumps and rocket engines [3, 4]. These exceptional properties, in combination with its thermal properties, makes SiC a promising substitute for traditional semiconductors, such as silicon, in high-temperature applications [5-12].

Silicon carbide nano layer (2D SiC) provides several advantages compared to the bulk silicon carbide, due to its two-dimensional structure. SiC is a promising nano material in optics, electronics, and optoelectronics industries [13-15]. The SiC layers can be grown exploiting both liquid and gas phase approaches [16]. Silicon carbide monolayer is a promising material in the semiconductor industry. The silicon and carbon elements in the two-dimensional silicon carbide are arranged in a two-dimensional hexagonal lattice [17].

To understand how heat spreads through a substance, we suppose heat (or sound) as the vibration of atoms and molecules. The quantum mechanics principles dictate that the vibrational energy (phonon energy) must be a multiple of a basic amount of energy and proportional to the frequency (https://news.mit.edu/2010/explained-phonons-0706). In the present study, the phonon density of states and phonon band structure of silicon carbide monolayer was investigated using first principles calculations. In this research, we intend to study the nano size effects on the vibration energies of a silicon carbide monolayer, and how it affects the energy states.

2. Materials and Methods

2.1 *Computational details*

The phonon properties of the SiC monolayer have been calculated by exploiting the DFT method as implemented in the SIESTA code. The calculation has been conducted via Generalized Gradient Approximation (PBE-GGA) to solve Kohn-Sham equations [18]. To reach energy eigenvalues convergence, the energy separating the core state from the valence state has been considered -9.0 Ry. Moreover, the magnitude of G_{max} (largest vector in charge density Fourier expansion) is optimized to 12 a.u.$^{-1}$. Figure 1 shows the crystal lattice of the silicon carbide monolayer. The carbon and silicon elements are represented by gray and yellow spheres, respectively. A tetragonal unit cell was chosen as the crystal lattice, in which x-direction has been selected as the normal vector of the plane. Besides, the k-point mesh (a finite number of points in the Brillouin Zone) was 25 × 25 × 1. The cell dimensions are as follows: a=b=10 Å, c=3.17 Å.

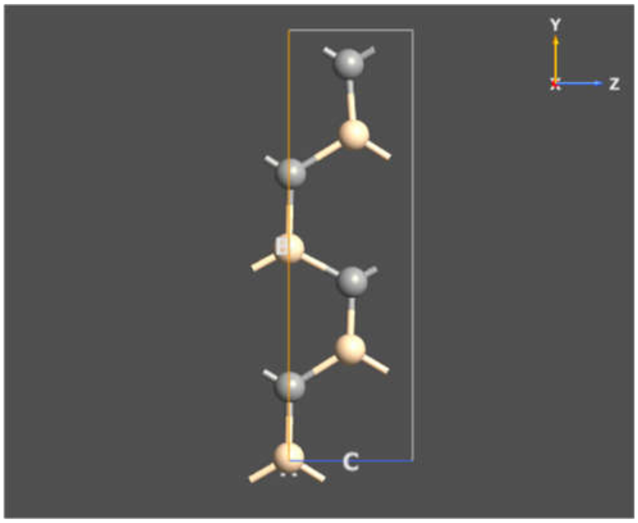

Figure 1. Crystal lattice of silicon carbide monolayer

3. Results and Discussion

The quantum of the crystal lattice vibrations, namely phonons, dominate mainly the physical characteristic of the crystals as a result of electron mobility. Figure 2 shows the phonon density of states (PDOS) of the silicon carbide monolayer. This parameter indicates the number of modes per unit frequency per the unit volume of real space [19]:

$$\mathrm{D_{Acoustic}}(\omega) = \frac{1}{\mathrm{L}^{\alpha=1}}\frac{\mathrm{dN}}{\mathrm{d}\omega} = \frac{1}{\mathrm{L}}\frac{\mathrm{dN}}{\mathrm{dk}}\frac{\mathrm{dk}}{\mathrm{d}\omega} = \frac{1}{\pi}\frac{1}{\mathrm{d}\omega/\mathrm{dK}} \tag{1}$$

$\mathrm{d}\omega/\mathrm{dK}$ is the e group velocity of acoustic phonons[20]:

$$\mathrm{D}(\omega) = \frac{1}{\pi \upsilon_g} \tag{2}$$

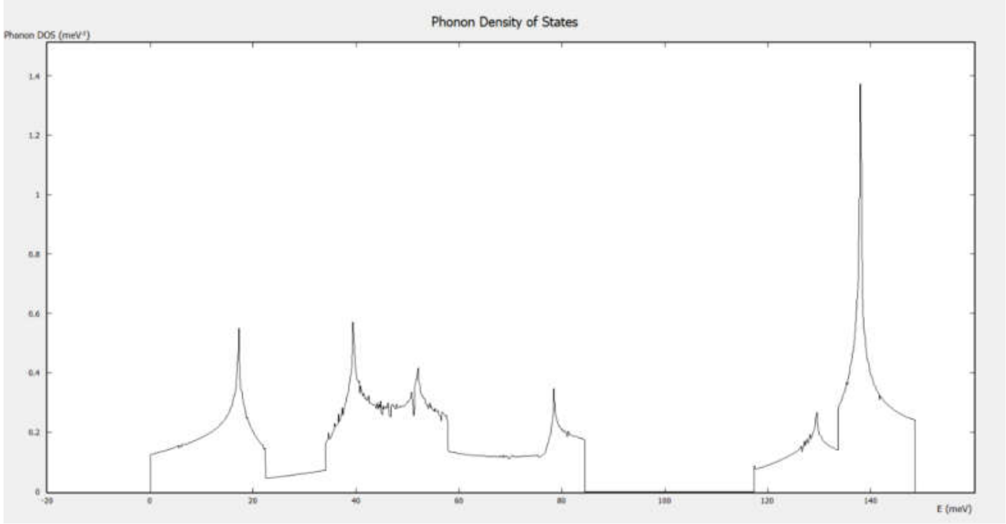

Figure 2. Phonon density of states (PDOS) of silicon carbide monolayer

Looking at Figure 2 and the phonon band structure in Figure 3, it is clear that the number of phonons is zero, from 85 meV to 117 meV. It is worth mentioning that because the number of phonons follows the Bose–Einstein distribution, the number of phonons occupied by each state represented in Figure 2 is a variable value. In addition, the silicon carbide monolayer sees its maximum at 140 meV, confirming that there are more allowed phonon energy levels at this point of energy. The energy states for vibration modes are a function of the number of atoms per unit cell, as well as the number of delocalized electrons.

Furthermore, there are four peaks from 0 meV to 85 meV, indicating optical phonons and zone boundary (ZB) phonons.

For the low-range energy, all electronic sub-bands (each energy band) correlate acoustic phonons, where the transverse acoustic phonons have lower energy than the longitudinal acoustic modes (see Figure 3).

On the other hand, the optical phonons have high energy ($\hbar\omega \sim 0.16$ eV [20]). Therefore, the electronic sub-bands (each energy band) with energies more than 0.16 eV are associated with optical and zone boundary phonons. As a matter of fact, the longitudinal optical modes have lower energy than the transverse optical (TO) ones [20].

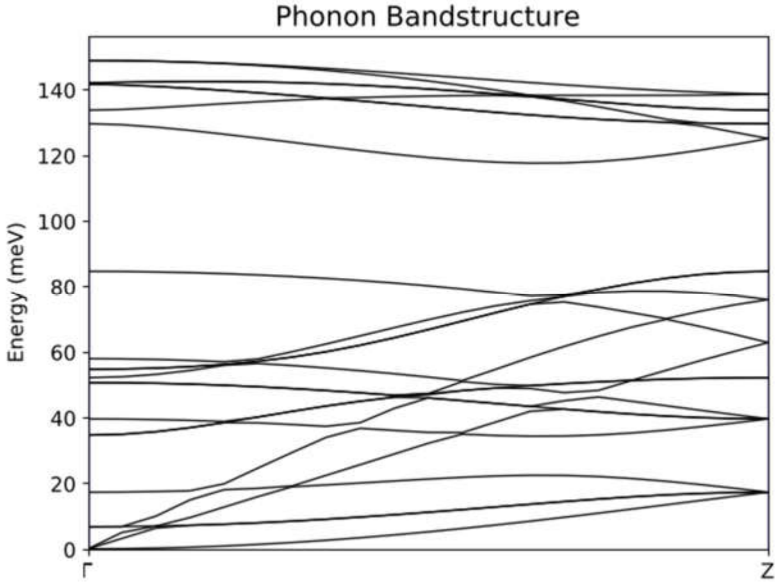

Figure 3. Phonon band structure of silicon carbide monolayer. The top lines of phonon band structures are related to the zone boundary and TO modes

4. Conclusions

The phonon properties of the SiC monolayer have been calculated by exploiting the DFT method as implemented in the SIESTA code. The calculation has been conducted via Generalized Gradient Approximation (PBE-GGA) to solve Kohn-Sham equations. The calculated number of modes per unit frequency per the unit volume of real space shows that there are four peaks from 0 eV to 85 eV, indicating optical phonons and zone boundary (ZB) phonons. For the low-range energy, all electronic sub-bands (each energy band) correlate acoustic phonons, where the transverse acoustic phonons have lower energy than the longitudinal acoustic modes. Our results show that the number of phonons is zero, from 85 meV to 117 meV. It is worth mentioning that because the number of phonons follows the Bose–Einstein distribution, the number of phonons occupied by each state represented in Figure 2 is a variable value.

Conflicts of Interest

The authors declare that they have no conflict of interest.

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