Electronic, thermal, and optical properties of graphene like SiC\(_x\) structures:
Significant effects of Si atom configurations

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Abstract

We investigate the electronic, thermal, and optical characteristics of graphene like SiC\(_x\) structure using model calculations based on density functional theory. The change in the energy bandgap can be tuned by the Si atomic configuration, rather than the dopants ratio. The effects of the concentration of the Si atoms and the shape of supercell are kept constant, and only the interaction effects of two Si atoms are studied by varying their positions. If the Si atoms are at the same sublattice positions, a maximum bandgap is obtained leading to an increased Seebeck coefficient and figure of merit. A deviation in the Wiedemann-Franz ratio is also found, and a maximum value of the Lorenz number is thus discovered. Furthermore, a significant red shift of the first peak of the imaginary part of the dielectric function towards the visible range of the electromagnetic radiation is observed. On the other hand, if the Si atoms are located at different sublattice positions, a small bandgap is seen because the symmetry of sublattice remains almost unchanged. Consequently, the Seebeck coefficient and the dielectric function are only slightly changed compared to pristine graphene. In addition, the electron energy loss function is suppressed in Si-doped graphene. These unique variations of the thermal and the optical properties of Si-doped graphene are of importance to understand experiments relevant to optoelectronic applications.

Keywords: Energy harvesting, Thermal transport, Optical properties, Graphene, Density Functional Theory, Electronic structure

1. Introduction

The discovery of carbon-related materials and their development has been considered to be crucial for the future of technology [1, 2, 3, 4, 5, 6]. Carbon based material such as monolayer graphene offers good possibility of device performance down to the atomic limit [7]. Extraordinary properties of graphene make it an interesting material for many electronic devices. The zero band gap of graphene leads it to be a metallic like material with non-trivial physical properties such as high electron mobility at room temperature and exceptional thermal conductivity [8]. The bandgap of graphene can be tuned by several techniques termed functionalization strategies [9], doping [10], application of an electric field [11] or a magnetic field [12], or strain [13], etc. Among these methods, the doping process is considered one of the most feasible ways to tune the bandgap of graphene and altering its physical characteristics, for the reason that doping can break or alter the symmetric structure of graphene [14].

The integration of two-dimensional graphene into silicon chips promises a better heterogeneous platform to deliver a massively enhanced potential based on silicon technology [15]. Silicon doped graphene systems (Si\(_x\)C\(_y\)) have emerged as new 2D materials called siligraphenes. They have been considered as good composite materials based on graphene to study enormously interesting physical application such as solar cell devices [16] and gas sensors [17]. Si-substituted graphenes have been identified as significant structures for technological application [18]. The ratio of the Si doping in graphene determines the potential or the functionality of the structure. For instance, SiC\(_2\) can be used to built solar cell devices due to its finite band gap [16], SiC\(_3\) and SiC\(_5\) can be used as topological insulators and semi-metals [17, 19], while SiC\(_7\) is suggested for photovoltaic devices [20, 21].

In recent years, the investigation of thermal properties of graphene like SiC\(_x\) structures (g-SiC\(_x\)) has been attracting the attention of many researchers, and the interest in the subject is still growing [22, 23]. It has been shown that the electrical and thermal properties of two configurations of siligraphene, g-SiC\(_3\) and g-SiC\(_7\) can be tuned by the concentration of the silicon. The thermal conductivity of g-SiC\(_7\) is exponentially enhanced with temperature, but it varies parabolically for g-SiC\(_3\) [24, 25]. Composite
thermal interface materials have been optimized with an admixture of graphene structures with different doped materials leading to a high enhancement of the effective thermal conductivity [5], which has been beneficial for large range of materials used by industry. Therefore, graphene based materials can be used for energy harvesting and increased efficiency of solar cell devices at room temperature due to a high-recorded thermal property dominated by the acoustic phonons [26].

Optical properties of g-SiC\(_x\) is another important aspect of research in which the g-SiC\(_x\) has been used for solar cell application. Optical properties such as the optical conductivity, reflectivity and refractive index have been studied and it has been demonstrated that the optical conductivity is enhanced due to the Si-dopant [27, 28]. Theoretical studies have shown that the bandgap of g-SiC\(_x\) is enhanced due to the Si-dopant [27, 28]. The imaginary part of dielectric function \(\varepsilon_{\text{imag}}(\omega)\), in the long wavelength limit, can be obtained directly from the electronic structure calculation

\[
\varepsilon_{\text{imag}}(\omega) = \left(\frac{4\pi\varepsilon_0^2}{\omega^2}\right)\sum_{i,j} \int (|M_{\text{cv}}(j)|^2 f_i(1 - f_j) \\
\times \delta(E_i - E_j - \omega) d^3k,
\]

where \(M_{\text{cv}}(k)\) are the dipole transition matrix elements [45].

3. Results

In this section, we present the main results calculated via DFT. We consider three Si doped graphene structures in addition to pure graphene (PG) as shown in Fig. 1(a-d). The three Si-doped graphene structures are: First, the two Si atoms (yellow) are doped at a para- and an ortho-position which means that the Si atoms are adjacent. The structure is identified as a g-SiC-1 (b). So, the two Si atoms are at different sublattice positions in which one dopant atom is placed at sublattice A and the other is at B. Second, the two Si atoms are put at the para- and the meta-position, i.e. the Si atoms are at the same sublattice positions (either A or B), forming g-SiC-2 (c). Finally, the
Figure 1: The $4 \times 4 \times 1$ supercell of PG (a), g-SiC-1 (b), g-SiC-2 (c), and g-SiC-3 (d) structures with their electron charge distribution (contour plot) are plotted. The corresponding band structure of four structures are shown from (e) to (h).

two Si atoms are both located at a para-position, resulting in g-SiC-3, shown in (d), in this case the two Si atoms are at different lattice positions [46, 47].

Among these Si-doped structures, g-SiC-1 seems to be less structurally stable compared to g-SiC-2 and g-SiC-3 since sp$^2$-hybridization is not favored by SiSi bonds, a planar structure should be energetically unfavorable [48].

The electron charge distributions of the four structures are plotted in Fig. 1 (contour plots). The high electron charge distribution between the carbon atoms in the PG indicates strong and stiff covalent bonds forming between the C atoms. Therefore, PG boasts of great stability and a very high tensile strength (the force with which one can stretch something before it breaks) [49]. In the g-SiC-1 structure, the Si atoms form Si-Si bonds and the electron charge distribution between the Si atoms is very weak because of the presence a strong repulsive force between the Si atoms. Furthermore, the C-Si bonds are somewhat polarized towards the C atoms due to carbon’s greater electronegativity. The electron charge distribution thus concentrates around the C atoms.

The same scenarios for electron charge distribution are also true for the other two Si-doped structures, g-SiC-2 and g-SiC-3. The electron charge distributions of all three Si-doped structures confirm that the C-Si bonds are longer and weaker than the CC bonds. This could be expected because of the larger atomic radius of a Si compared to a C atom.

Electronic band structure is calculated along the high-symmetry Γ-K-M-Γ directions. By looking at the band structures, we can see that the conduction and valence bands touch at the Fermi level, zero energy, as is presented in Fig. 1(e) for PG. One can see from the band structures in Fig. 1(fh) that the maximum band gap appears for g-SiC-2 and it is equal to 0.358 meV. The category of g-SiC-2 originates when both the Si dopants are placed at the same sublattice positions (either A or B). This observation confirms that the origin of the bandgap is due to symmetry breaking of graphene sublattices, which is maximized in these configurations. The same scenario has been seen for Boron or Nitrogen doped graphene [46].

3.1. Thermal properties

We display thermoelectric properties at 100 K which is in the intermediate temperature range, 50-160 K, where the electron and the lattice temperatures are decoupled. The electronic thermal conductivity $k_e$ is thus proportional to the charge conductivity at a given temperature. In this temperature range, the electron and the lattice temperatures are very well decoupled in low-disorder graphene [50, 51].

Figure 2 shows the contributions of the electrons to different thermoelectric parameters, the Seebeck coefficient (a) and the figure of merit (b). In general, semiconductor materials with high a bandgap effectively minimize free charge carrier contributions. The Seebeck coefficient is thus enhanced since $S$ is inversely proportional to charge carrier concentration [52]. The Seebeck coefficient is found to be significant and as high as 1.67 mV K$^{-1}$ for g-SiC-2 (green line), i.e. higher than the value of 6 µV K$^{-1}$ for PG. The enhancement of the Seebeck coefficient is attributed to the existence of the high bandgap of g-SiC-2 compared to PG. In addition, the Seebeck coefficient of g-SiC-1 and g-SiC-3 is smaller than that of g-SiC-2 due to the smaller bandgaps of these two structures.

Figure of merit is what ultimately would determine the efficiency of the devices. It is interesting to compare the $ZT$ of the four aforementioned structures. One can see that increased Seebeck coefficient raises the enhancement of figure of merit as is presented in Fig. 2(b), where the maximum $ZT$ is found for g-SiC-2 (green line).

We now consider the Wiedemann-Franz (WF) law for our model. The WF law states that the ratio of $k_e$ to $\sigma$ is given by

$$\frac{k_e}{\sigma} = LT$$

(5)
Figure 2: The Seebeck coefficient, $S$, (a) and the figure of merit, $ZT$, (b) at intermediate temperature $T = 100$ K for PG (brown), g-SiC-1 (blue), g-SiC-2 (green) and g-SiC-3 (red).

which is constant for ordinary metals, where $L = L_0 = \pi^2 k_B^4/3e^2 = 2.44 \times 10^{-8}$ W Ω K$^{-2}$, called the Lorenz number [53, 54]. For graphene, the low chemical potential makes the Lorenz number sensitive to resonance scattering and the energy dependence of the relaxation time [55]. Figure 3 displays the Lorenz factor for all four structures shown in Fig. 1 at the intermediate temperature $T = 100$ K. It can clearly be seen that $L$ strongly depends on the energy or chemical potential, especially around the resonance states. In addition, the value of $L$ depends on the location of the resonance states of the different Si atomic configuration in our calculations. The maximum value of $L = 3.62 \times 10^{-6}$ W Ω K$^{-2}$ is found for g-SiC-2. We conclude that the WF law is not obeyed in our Si-doped graphene structures at $T = 100$ K [50].

Figure 3: The Lorenz number, $L$, at the intermediate temperature $T = 100$ K for PG (brown), g-SiC-1 (blue), g-SiC-2 (green) and g-SiC-3 (red).

3.2. Optical properties

Graphene has unique optical characteristics and can absorb a wide range of electromagnetic radiation [56]. PG is known to emit light when it has been excited by a near-infrared laser [57]. In the case of doped graphene, photoluminescence is observed by creation of a bandgap [58].

We use the three aforementioned silicon atom configurations to investigate the optical properties of doped graphene. The imaginary part of the dielectric function, $\varepsilon_{\text{imag}}(\omega)$, is presented in Fig. 4 for PG (brown), g-SiC-1 (blue), g-SiC-2 (green), and g-SiC-3 (red) in the case of parallel (a) and perpendicular (b) electric field. In the case of PG, two peaks in the imaginary part of dielectric function for a parallel electric field are observed (brown line), one at 4.0 eV indicating $\pi \rightarrow \pi^*$ transition and another at 14.0 eV displaying $\sigma \rightarrow \sigma^*$ transition. The position of both peaks in our calculation is in a good agreement with the literature [59, 60]. The intensity ratio of these two peaks is $\varepsilon_{\text{imag},L}/\varepsilon_{\text{imag},R} = 2.82/2.092 = 1.34$ demonstrating that the $\pi \rightarrow \pi^*$ transition is stronger than the $\sigma \rightarrow \sigma^*$ transition. This is what should be obtained for monolayer pure graphene. In the case of a perpendicular electric filed Fig. 4(b), two main peaks for PG appear at 11.06 and 14.42 eV belonging to the $\pi \rightarrow \sigma^*$ and the $\sigma \rightarrow \pi^*$ transitions, respectively.

Figure 4: The imaginary part of dielectric function, $\varepsilon_{\text{imag}}(\omega)$, is plotted for PG (brown), g-SiC-1 (blue), g-SiC-2 (green), and g-SiC-3 (red) in the presence of a parallel (a) and a perpendicular (b) electric field.

Let’s look at the effect of silicon doping of graphene on the imaginary part of dielectric function. It is interesting to see an extra peak at 0.4 eV, in the visible range, in the case of a parallel electric field for g-SiC-2 (see the inset of Fig. 4(a)) [61]. The extra peak can be referred to the
existence of a finite bandgap. Our analysis shows a significant red shift of the first peak of the dielectric function towards the visible range. The peak structure becomes more complex due to the Si doping, and more peaks may be identified in the visible range. Furthermore, the intensity of both peaks is decreased in the case of Si-doping for perpendicular electric field as is shown in Fig. 4(b). This indicates that both transitions, $\pi \rightarrow \sigma^*$ and $\sigma \rightarrow \pi^*$, are weaker compared to the corresponding transitions active in PG. These unique variations of the dielectric function of Si doped graphene are of importance to understand relevant experiments and design for optoelectronic applications [62, 63].

The electron energy-loss function (EELF) is shown in Fig. 5 in the presence of parallel (a) and perpendicular (b) electric field for PG (brown), g-SiC-1 (blue), g-SiC-2 (green), and g-SiC-3 (red). The electron inelastic interaction with a structure is closely related to the EELF which represents the probability of inelastic scattering events. It can clearly be seen that the EELF is decreased for all three Si-doped graphene structures. This is attributed to the low probability of charge concentration close to a Si-dopant in Si-doped graphene structures. This is attributed to the low probability of charge concentration close to a Si-dopant in the graphene nanosheets [60]. It should be mentioned that EELS obtains a maximum value where $\varepsilon_{\text{imag}}(\omega)$ has a finite small value. So, plasmonic excitations can be responsible for the maximum intensity of EELS peak [64].

4. Conclusion

In summary, the characteristics of monolayer graphene-like materials with $\text{SiC}_x$ stoichiometry are investigated where the position of the Si atoms plays an important role for their physical properties. The electronic band structure of graphene can be remarkably modulated by different Si doping configurations, leading to Dirac point shifting and even opening of bandgaps. Consequently the figure of merit is enhanced. In addition, the optical properties, such as the dielectric and the electron energy loss function are influenced by the tuning of the bandgap. As a result, a reduction in electron energy loss function has been found, and an extra peak in imaginary part of the dielectric function towards the visible range is found. Last but not least, we show that our model does not obey the Wiedemann-Franz law. Therefore, a maximum value of Lorenz number is found around resonant scattering states.

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