Outstanding tunable electrical and optical characteristics in monolayer silicene at high terahertz frequencies

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Abstract
Silicene, a zero-bandgap semimetallic advanced material, has received much attention due to its extraordinary electronic and optical characteristics, enabling its use in plasmonic nano-devices. This material is able to be tuned without degrading its high carrier mobility. In this work, by applying rigorous numerical techniques, the optical and electrical properties of silicene at high terahertz frequencies are calculated. Under the influence of environmental effects including the Fermi level, temperature, and external electric field, the optical conductivity and refractive index of silicene are investigated using the tight-binding model. The effects of the Fermi level from 0 to 1 eV, the external electric field from 0 to 2.5 V/A, and temperature from 5 to 400 K are investigated with respect to the optical properties of silicene. One of the interesting features of silicene is its adjustable bandgap, which we present here.

Keywords Silicene · Tunable optical properties · Terahertz properties

1 Introduction
Because of their attractive structure, two-dimensional (2D) materials have long been of interest to researchers. Many-layer materials have very strong intra-plate chemical bonds, but their inter-layer coupling is poor. As a result, these multi-layered structures can break down and become single layers. Thus they are converted into 2D materials due to their limitations in one direction. A 2D material with amazing properties that has been discovered in recent decades is graphene [1]. The valence and conduction bands of graphene touch each other at the Dirac point (k in the Brillouin zone). At this point, the number of electronic states is low, so graphene is known as a semiconductor with a zero bandgap. The presence of this zero bandgap allows the absorption of light in a wide range from infrared to ultraviolet [2]. The discovery of graphene sparked much interest in exploring other 2D materials such as silicene [3], germanene [4], stanene [5], phosphorene [6], boron nitride [7], two-dimensional MXC3 [8], 2D penta-Pt2N4 monolayer [9], and penta-MP2 monolayer [10]. Among these materials, silicene has been considered because of its compatibility with current technology, as well as its very interesting electrical and optical properties [11]. In 1964, Hohenberg and Kohn showed that, in terms of energy for silicene, a buckled structure is more appropriate than a flat structure (such as the graphene structure). The band structure of silicene was also investigated, but there was no emphasis on Dirac cones [12]. This theoretical study was disregarded for about a decade, for two reasons. First, there was a common belief that these 2D materials could not exist [13, 14]. Second, it was difficult to believe that silicone could create an sp2 hybridization, as it always prefers sp3 hybridization [15]. The electronic and atomic structure of the material that is now known as silicene was first introduced by Takeda and Shiraishi in 1994 [16]. In 2005, Léandri et al. synthesized silicene on a silver substrate [17]. The flat structure of silicene was also proposed by Guzmán-Verri and Voon in 2007 using a tight-binding (TB) model [18]. It was emphasized that, similar to graphene, the flat structure of silicene also displays linear cross-bands at the Fermi level. The name “silicene” was first used in that study. It was later discovered that the flat silicene was unstable and that the only stable silicene structure was the low-buckled. Silicene features are more interesting than graphene features. The first feature is that its bandgap can be adjusted with an external electric field, and thus it can be used to fabricate field-effect transistors at room temperature [19]. The second
feature is the stronger spin–orbit coupling, so the quantum spin Hall effect can be seen even at high temperatures [20]. Currently, there is much research on the structure and electrical, optical, and mechanical properties of silicene. One of the hottest topics is the finding of sublayers that silicene can be grown on, so that, firstly, its structure remains stable and, secondly, it preserves the Dirac states [21]. Silicene has been successfully grown on metal substrates such as Ag(111) [22], Ir(111) [23] and ZrB2(0001) [24]. Silicene can also be grown on a nonmetallic aluminum substrate of Al2O3 that maintains the structural profile of a low-buckled honeycomb lattice [25]. More recently, graphene [26] and silicane [27] substrates have also been studied. Numerous articles have reported on the electrical properties of silicene and examined the effects of electric and magnetic fields on its electrical properties [28–30]. Because of the adjustability of the bandgap of silicene with the electric field, it has been used in the field-effect transistor channel [31–33]. Another potential application of silicene is in gas detection sensors, which are much more sensitive and smaller than conventional semiconductor sensors [34, 35]. There are also limited studies on the optical properties of silicene, and research is still ongoing on its optical properties. In [36] the optical properties of 2D materials including graphene, silicene, germanene, and stanene were examined in a range from the infrared to ultraviolet. Chowdhury et al. [37] examined the effects of electric and magnetic fields on the optical properties of silicene. Also, Bao et al. [38] reported on the optical properties of silicene nanoribbons and the effect of an external field. Other articles have investigated the optical properties of silicene [39–42]. In this paper, we explore the optical properties of silicene, namely optical conductivity and refractive index, under the influence of environmental factors including temperature, Fermi level, $E_F$, and external electric field, $E_z$, perpendicular to it.

2 Fundamental data

Silicene is a monolayer of silicon atoms arranged in the form of a honeycomb. Of all the flat, low-buckled, and high-buckled silicene structures studied, only the low-buckled structure is stable [41]. Figure 1a illustrates the silicene honeycomb lattice and Fig. 1b shows the side view with a buckling height equal to $d$. Unlike graphene, whose atoms are on the same plane, due to the tendency toward sp$^3$ hybridization, silicene atoms are not located on one plane.

\[
H_{\text{eff}} = \begin{pmatrix}
\Delta_{\text{eff}} & h\nu_F (\eta k_x - i k_y) \\
h\nu_F (\eta k_x + i k_y) & -\Delta_{\text{eff}}
\end{pmatrix} = h\nu_F (\eta k_x \tau_x + k_y \tau_y) + \Delta_{\text{eff}} \tau_z
\]

\[
\Delta_{\text{eff}} = \eta \mu \lambda_{\text{SO}} - E_z d
\]

The inherent structure of silicene has two exceptional features. The first is a strong spin–orbit (SO) coupling that turns the silicene into a topological insulator [43]. The second interesting feature is the buckled structure. When a perpendicular external electric field, $E_z$, is applied to the surface of silicene, a potential difference is created between the two A and B sub-lattice atoms and changes the bandgap. As a result, silicene has a bandgap that can be adjusted by $E_z$.

The silicene TB model can be described as [44]

\[
\hat{H}_0 = -t \sum_{\langle ij \rangle} \hat{c}_i^\dagger \hat{c}_j + \frac{i \lambda_{\text{SO}}}{3\sqrt{3}} \sum_{\langle ij \rangle, \langle kl \rangle} \langle s \rangle_{ij} \langle c \rangle_{jl} - \sum_i \langle s \rangle_i \hat{E}_z \hat{c}_i^\dagger \hat{c}_j
\]

\[
(1)
\]

where, compared to the Hamiltonian of graphene [45], it has two more terms because of the strong SO coupling and the buckled structure of silicene. The first term expresses the interactions of the nearest neighbors with the transfer energy, $t$. The second term considers the effects of SO coupling with strength $\lambda_{\text{SO}} = 3.9 \text{ meV}$. The third term represents the potential difference between the two sub-lattices due to the external electric field, $E_z$. The behavior of electrons in low-energy physics can be approximated by Dirac cones (points $k$ and $k'$ in the Brillouin zone). The Hamiltonian of silicene at these points is as follows:

\[
\Delta_{\text{eff}} = \eta \mu \lambda_{\text{SO}} - E_z d
\]
index related to the valleys, which is positive for \( k \) valleys and negative for \( k' \) valleys, \( v_F \) is the Fermi velocity, equal to \( 5.5 \times 10^5 \) m/s, and \( \Delta_m \) refers to the size of the bandgap. By solving Eq. (2) and obtaining its eigenvalues, the energy dispersion for \( \eta \)-valley and \( s \)-spin is obtained as

\[
E_{\eta}(k) = \pm \sqrt{(h v_F k)^2 + (\Delta_m)^2}
\] (4)

\[
k = \sqrt{k_x^2 + k_y^2}
\] (5)

Figure 2 shows the dispersion of the electric field at the \( k \) point and \( k' \) point for different values of \( E_z \). The red lines are related to the spin-up electron scattering and the blue dotted lines are related to the spin-down electron scattering. In \( E_z = 0 \), the two bands overlap, and as \( E_z \) increases, the two bands separate and a bandgap is formed (Fig. 3).

3 Method for calculating the surface conductivity of silicene

In this essay, we have analytically calculated the surface conductivity of silicene (\( \sigma_{\eta}(\omega) \)) using the Kubo formulation, and we used Wolfram Mathematica 11.3 software to simulate and obtain the results. According to this model, the optical conductivity can be written as [46]

\[
\sigma_{\eta}(\omega) = -\frac{i e^2}{4 \pi \hbar^2} \left( \sum_k \int d^2k (v_{s1}^\prime)^2 \frac{d[f(e_{s1})]}{de_{s1}} \right)
\]

\[
+ \frac{i \omega e^2 \hbar^2}{2 \pi} \left( \int d^2k \frac{f(e_{s1}(k)) - f(e_{s2}(k))}{e_{s2}(k) - e_{s1}(k)} \right) \frac{v_{s1}^\prime v_{s2}^\prime}{\hbar^2 \omega^2 - (e_{s1}(k) - e_{s2}(k))^2}
\]

(6)

where \( \omega \) is the angular frequency, \( f(\epsilon) \) is a Fermi distribution function equal to \( f(\epsilon) = \left( 1 + e^{-\frac{\epsilon - E_F}{kT}} \right)^{-1} \), where \( E_F \) is the Fermi level, \( e \) is the Boltzmann constant and \( T \) is the temperature. \( v_{s1}^\prime \) is the element of the velocity matrix. By solving Eq. (6), the conductivity of silicene is calculated as \( \sigma = \sigma_{\text{ intra}} + \sigma_{\text{ inter}} \).

\[
\sigma_{\text{ intra}} = \int \frac{i e^2}{4 \pi \hbar^2} \left( \frac{\left( E_F + \frac{\hbar \omega}{e} \right)^2}{\left( E_F + \frac{\hbar \omega}{e} \right) \left( \omega + \frac{\pi}{\hbar} \right)} \right) + \frac{i e^2}{4 \pi \hbar^2} \left( \frac{\left( E_F + \frac{\hbar \omega}{e} \right)^2}{\left( E_F + \frac{\hbar \omega}{e} \right) \left( \omega + \frac{\pi}{\hbar} \right)} \right) \frac{1}{\hbar^2 \omega^2 - (e_{s1}(k) - e_{s2}(k))^2} \frac{d\epsilon}{\Gamma}
\]

(7)

Fig. 2 Electronic energy band structure of silicene at the \( K \) valley
In the above equations, \( d = 0.46 \) Å is the vertical distance of the atoms of the sub-lattices A and B of silicene. \( \Gamma = 10^{-5} e \) is the phenomenological scattering rate at which \( e = 1.6 \times 10^{-19} \) is the charge of an electron. \( \theta \) is a Heaviside function which is defined as follows:

\[
\theta(\omega, \xi, \eta) = \begin{cases} 
0 & \text{if } \hbar \omega < \Delta[\xi, \eta] \\
1 & \text{else}
\end{cases}
\]

By computing the optical conductivity, we can determine the dielectric function and refractive index of silicene with a thickness of \( \Delta = 0.4 \) nm.

\[
\epsilon = 1 + \frac{i \sigma(\omega)}{\epsilon_0 \omega \Delta}
\]

\[
\epsilon = \epsilon' + i \epsilon''
\]
4 Results and discussion

4.1 The effect of Fermi level ($E_F$) on the optical properties

In this section, we evaluate the effects of the Fermi level $E_F$ on silicon optical conductivity, $\sigma(\omega)$, and refractive index, $N(\omega)$. Figure 4 shows the real and imaginary parts of the optical conductivity of silicene in the terahertz regime at 300 K for different values of the Fermi level from 0 to 1 eV. As $E_F$ increases, the real part of $\sigma(\omega)$ shifts toward higher frequencies. Also, with the shift to higher frequencies, larger negative values are achieved. This makes it possible to obtain a suitable and wide range for the propagation of TE waves by controlling $E_F$.

\[ N = \sqrt{\varepsilon} = n + ik \]  
(12)

\[ n = \sqrt{\frac{\varepsilon' + \varepsilon'' + \varepsilon'}{2}} \]  
(13)

\[ k = \sqrt{\frac{\varepsilon' + \varepsilon'' - \varepsilon'}{2}} \]  
(14)

Fig. 4 a Real and b imaginary parts of silicene optical conductivity, $\sigma(\omega)$, at different Fermi levels

Fig. 5 a Real and b imaginary parts of the silicene refractive index versus frequency at different Fermi levels

Fig. 6 a Real and b imaginary parts of the silicene optical conductivity, $\sigma(\omega)$, versus frequency, at different external electric fields

Fig. 6 a Real and b imaginary parts of the silicene optical conductivity, $\sigma(\omega)$, versus frequency, at different external electric fields.
Figure 5 shows the real and imaginary parts of the refractive index of silicene for different Fermi levels. As the Fermi level increases, the amplitude decreases, and its peak shifts toward higher frequencies. The same effects are seen on $k$, and it becomes zero at some frequencies for $E_F > 0.6$ eV. This indicates that the optical losses of the silicene layer will be zero.

4.2 The effect of external electric field, $E_z$, on the optical properties of silicene

As mentioned, in addition to $E_F$, the optical properties of silicene can be controlled by applying an electric field $E_z$. Figure 6 shows the effect of the electric field $E_z$ on the real and imaginary parts of the optical conductivity up to 2.5 V/Å at 300 K. The structure of silicene can withstand an external electric field $E_z$ up to 2.6 V/Å but will be unstable at higher fields [47]. For $E_z > 0.5$ V/Å, in addition to the
shift, the amplitude of the real part increases. Moreover, an amount increase in $E_z$ causes the amplitude and the range in which the imaginary part of $\sigma(\omega)$ has a negative value to increase. As a result, we have a wider range for TE wave propagation. Compared to the effects of $E_F$, here the range of negative values is larger.

Figure 7 shows the effects of $E_z$ at 300 K on the refractive index. As $E_z$ increases, the peak of $n$ shifts toward higher frequencies, and its amplitude decreases. Compared to the effects of $E_F$, here we will obtain a larger $n$ amplitude. We have the same effects on $k$, the only difference being that as $E_z$ increases, the frequency range in which $k \approx 0$ expands.

4.3 Temperature effects

Temperature can also affect the optical properties of silicene. Figure 8 shows the effects of temperature variation on the silicene conductivity, $\sigma(\omega)$, for $E_z=0.1$ V/Å and $E_F=0$ eV. At temperatures of 5 to 50 K, the effects of temperature on the real and imaginary parts are very insignificant. The black line indicates the conductivity variation at 5 K and the red line shows it at 50 K, which are almost identical. At a higher temperature, the amplitude of the conductivity peak is reduced. The thermal effects on the imaginary part of the optical conductivity are significant as well. As can be seen from Fig. 8, by increasing the temperature, the magnitude of the negative values of the imaginary part is reduced, so that at 400 K we have almost no negative value.

The effect of temperature on the silicene refractive index is shown in Fig. 9. When the temperature increases, the amplitude of the real part of the refractive index decreases, as shown in Fig. 9a. Also, Fig. 9b shows the effects of temperature on the imaginary part of the refractive index.

4.4 Optical properties at a wavelength of 1550 nm

In this section, we present the effects of the Fermi level and the external electric field at room temperature and a wavelength of 1550 nm. Figure 10 shows the effect of the variations in Fermi energy at a wavelength of 1550 nm on the silicene optical conductivity. The real part of the silicene optical conductivity up to 300 meV is almost constant and is equal to 0.06 mS, and at 500 meV this value becomes negligible. The effect of the Fermi level on the imaginary part of the silicene optical conductivity is slightly different, as can be seen in Fig. 9. For values above 200 meV, the imaginary part becomes negative, and at 400 meV, one can see the maximum negative amplitude. With further enhancement of the Fermi level, the value of the imaginary part changes from negative to positive. Figure 11 shows the effects of the Fermi level on the silicene refractive index at a wavelength of 1550 nm and room temperature, 300 K. As can be seen, the maximum amplitude of the real refractive index occurs at a Fermi level of about 400 meV, which is equal to 3.3. As the Fermi level further increases, the amplitude of the real part of the refractive index decreases, and at higher than 500 meV is almost negligible. Also, at a Fermi level of around 500 meV, the amplitude of the imaginary part of the silicene refractive index reaches its lowest value, and with an increase in the Fermi level, it increases.

Fig. 11 Effect of variation in Fermi level on real and imaginary parts of silicene refractive index at a wavelength of 1550 nm

Fig. 13 Effect of external electric field on the refractive index of silicene at a wavelength of 1550 nm
Figure 12 shows the effect of the external electric field on the optical conductivity of silicene at a wavelength of 1550 nm and room temperature, 300 K. According to the results, the maximum magnitude of the real part occurs at 1700 mV/Å, equal to 0.12 mS, and the lowest magnitude of the imaginary part is created at 1800 mV/Å, which is equal to −0.2 mS. Figure 13 shows the effects of the electric field on the refractive index of silicene. The highest magnitude of the real part of the refractive index occurs at 1800 mV/Å and is equal to 7, which is about twice as large as the peak in the Fermi level effects.

5 Conclusion

In this work, we examined the optical properties of silicene under the effects of the Fermi level, the external field perpendicular to the silicene surface, and the temperature. We presented the results of the Fermi level changes in the range of 0 to 1 eV, taking into account an external field of 0 V/Å and a temperature of 300 K. We also examined the effects of the external field in the range of 0 to 2.5 V/Å with a Fermi level of 0 eV and temperature of 300 K. We showed the effects of temperature in the range of 5 to 400 K on the optical properties of silicene. Also, we further investigated the effects of the Fermi level and external field on the optical conductivity and refractive index of silicene at a wavelength of 1550 nm. The results showed that the effects of the external electric field were greater than those of the Fermi level. The authors declare that there is not conflict of interest.

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