Outstanding Tunable Electrical And Optical Characteristics In Monolayer Silicene At high Terahertz Frequencies

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Outstanding Tunable Electrical and Optical Characteristics in Monolayer Silicene at high Terahertz Frequencies

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Abstract

Silicene, a zero-gap semi-metallic advanced material, has received much attention due to its extraordinary electronic and optical characteristics, which could be used in plasmonics nano-devices. This material presenting as a tunable material without degrading its high carrier mobility. By applying the rigorous numerical techniques, the optical and electrical properties of silicene at high terahertz frequencies are calculated here. Beneath the influence of environmental effects such as the Fermi level, temperature, and external electric field, on the optical conductivity and refractive index of silicene are investigated using the tight-binding model. The effect of Fermi level from zero to 1 eV, external electric field from zero to 2.5 eV, and temperature from 5 to 400 K are investigated on the optical properties of silicene. One of the interesting features of Silicene is its adjustable bandgap, which we are present here.

Keywords: Silicene, Tunable optical properties, Terahertz properties

1. Introduction

Due to their attractive structure, two-dimensional (2D) materials have always been of interest to researchers. Many layered materials have very strong intra-plate chemical bonds, but instead, their inter-layer coupling is poor. As a result, these layered structures can break down and become single layers. These layers are converted into 2D materials due to their limitations in one direction. In recent decades, one of the 2D materials with amazing properties that has been discovered is graphene [1]. The valence and conduction bands of the graphene touch each other at 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 band gap allows the absorption of light in a wide range from infrared to ultraviolet [2]. The discovery of graphene aroused many motivation to research other 2D materials Such as Silicene [3], germanene [4], stanene [5], phosphorene [6], nitride boron [7], etc. Among these materials, Silicene was taken into consideration due to its compatibility with current technology, as well as its very interesting electrical and optical properties [8]. 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 presented, but there was no emphasis on Dirac's cones [9]. The mentioned theoretical study was disregarded for about a decade for two reasons. First, there was a common belief that these 2D materials could not exist [10-11]. Second, it's hard to believe that silicone will be able to create a sp^2 hybridization, as it always prefers sp^3 hybridization [12]. The electronic and atomic structure of a matter that is now known as Silicene, was first introduced by Takeda and Shiraishi in 1994 [13]. In 2005, Léandri et al. has synthesized the Silicene on the silver substrate [14]. The flat structure of Silicene was also proposed by Guzmán-Verri and Lew Yan Voon in 2007 using a tight-binding (TB) model. The flat structure of Silicene was also proposed by Guzmán-Verri and Lew Yan Voon in 2007 using a tight-fitting model [15]. In this study, 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 this study. It was later discovered that the flat Silicene was unstable and the only stable structure of the Silicene was the low buckled. Silicene features are interested rather than graphene features. The first feature is that its bandgap can be adjusted with an external electric field, which can be used to make field-effect transistors at room temperature [16]. The second feature is the stronger spin-orbit coupling, so the quantum spin Hall Effect can be seen even at high temperatures [17]. Currently, there is a lot of research on the structure and electrical, optical, and mechanical properties of Silicene. One of the hottest topics is the finding of sub-layers that Silicene can be grown on it, so that, firstly, its structure remains stable and, secondly, it preserves the Dirac states [18]. Silicene has been successfully grown on metal substrates such as $Ag(111)$ [19], $Ir(111)$ [20] and $ZrB_2(0001)$ [21]. Silicene also can be grown on a non-metallic aluminum substrate of Al_2O_3 that maintains the structural profile of low-buckled honeycomb lattice [22]. More recently, the graphene [23] and the silicane [24] substrates have also been studied. Numerous articles have worked on the electrical properties of silicene and examined the effects of electric and magnetic fields on the electrical properties of silicene [25-27]. Due to the adjustability of the bandgap of Silicene with the electric field, it has been used in the field-effect transistor channel [28-30]. Another potential application of silicene is the gas detection sensors, which are much more sensitive and smaller than conventional semiconductor sensors [31-32]. There are also limited studies on the optical properties of silicene and research is still ongoing on its optical properties. In [33] the optical properties of 2D materials such as graphene, silicene, germanene, and stanene are examined in the range of IR to UV. Article [34] also examine the effects of electric and magnetic fields on the optical properties of silicene. Also in [35] have been worked on the optical properties of silicene nanoribbons and the effect of an external field on them. Other articles have investigated the optical properties of silicene [36-39]. In this paper, we explore the optical properties of silicene such as optical conductivity and refractive index under the influence of environmental factors such as temperature, Fermi level, E_F, and perpendicular external electric field, E_z 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 studied silicene structures, only the low-buckled structure is stable [38]. Fig. 1(a) illustrates the silicene honeycomb lattice and Fig. 1(b) shows the side view with a buckling height equal to "d". Unlike graphene, whose atoms are on the same plane, due to the tendency to sp^3 hybridization, silicene atoms, are not located on one plane. The inherent structure of silicene has two marvelous features. The first is a strong spin-orbit (SO) coupling that turns the silicene into a topological insulator [40]. 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 changed the bandgap of silicene. As a result, Silicene has a bandgap that can be adjusted by E_z.

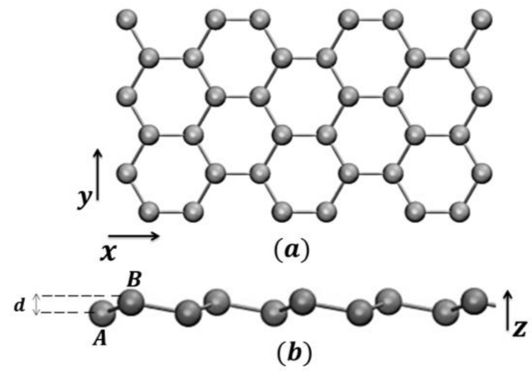

Fig. 1. (a) Top view and (b) side view of Silicene honeycomb structure [38].

The silicene tight binding (TB) model can be stated as [41]:

$$\widehat{H_0} = -t\sum_{<i,j>s} c_{is}^{\dagger}\ c_{js} + i\frac{\lambda_{SO}}{3\sqrt{3}}\sum_{\ll i,j\gg s} s v_{ij}\ c_{is}^{\dagger} c_{js} - l\sum_{is}\mu_i E_z c_{is}^{\dagger} c_{js} \quad (1)$$

that compared to Hamiltonian of graphene [42], it has two more terms because of the strong SO coupling and the buckled structure of the 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 λ_{SO}=3.9 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 physic can be approximated by Dirac's cones (points k and k' in the Brillouin zone). The Hamiltonian of silicene at these points is as follows:

$$H_{s\eta} = \begin{pmatrix} \Delta_{s\eta} & \hbar v_F(\eta k_x - ik_y) \\ \hbar v_F(\eta k_x + ik_y) & -\Delta_{s\eta} \end{pmatrix} = \hbar v_F(\eta k_x \tau_x + k_y \tau_y) + \Delta_{s\eta}\tau_z \tag{2}$$

$$\Delta_{s\eta} = \eta s \lambda_{so} - E_z d \tag{3}$$

The Dirac points are labeled with two parameters $s = \pm$ and $\eta = \pm$, where *s* is the valley index, positive for spin-up electron and negative for spin-down electron. Also η is an index related to the valleys, which is positive for k valley and is negative for k' valley, and v_F is the Fermi velocity, equal to 5.5×10^5 m/s and $\Delta_{s\eta}$ refers to the amount of the bandgap. By solving Eq. 2 and obtaining its eigenvalues, the energy dispersion for η-valley and *s*-spin is obtained as:

$$E_{s\eta}(k) = \pm\sqrt{(\hbar v_F k)^2 + (\Delta_{s\eta})^2} \tag{4}$$

$$k = \sqrt{{k_x}^2 + {k_y}^2} \tag{5}$$

Fig. 2 shows the dispersion of the electric field at 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 are overlapped and as E_z increases, the two bands will be separated, and a bandgap is formed.

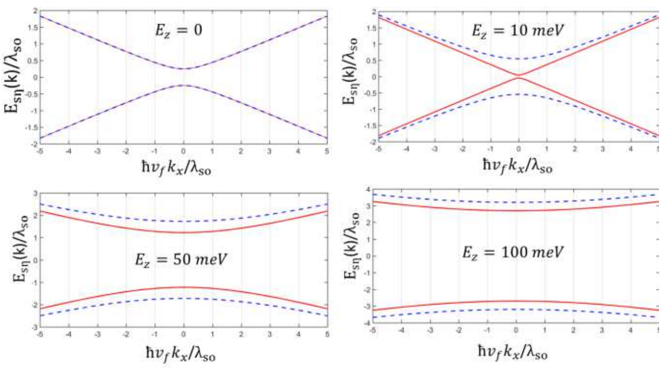

Fig. 2. Electronic energy band structure of silicene at *K* valley.

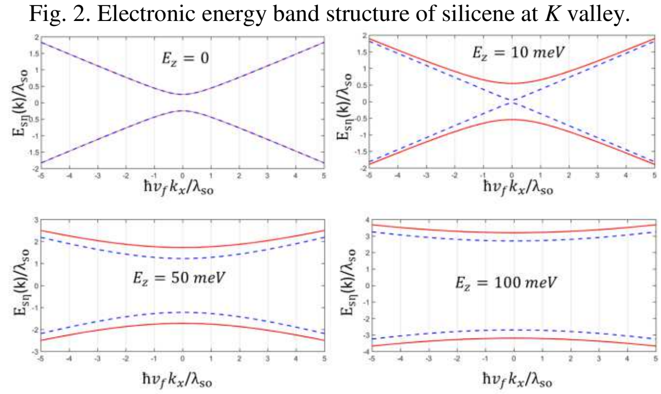

Fig. 3. Electronic energy band structure of silicene at K' valley.

We used the Kubo model to obtain the optical properties of silicene. According to this model, the optical conductivity can be written as [43]:

$$\sigma_{s\eta}(\omega) = -\frac{ie^2}{4\omega\pi^2}\left(\sum_s \int d^2k (v_{ss}^x)\frac{df[\epsilon_{s\zeta\eta}]}{d\epsilon_{s\zeta\eta}}\right) + \frac{i\omega e^2}{2\pi^2}\hbar^2(\int d^2k \frac{f[\epsilon_{1s\eta}(k)]-f[\epsilon_{2s\eta}(k)]}{\epsilon_{2s\eta}(k)-\epsilon_{1s\eta}(k)} \frac{v_{12}^x v_{21}^x}{\hbar^2\omega^2-[\epsilon_{2s\eta}(k)-\epsilon_{1s\eta}(k)]^2} \tag{6}$$

Where f is the Fermi distribution function and v_{ss}^{x} is the velocity matrix element. By computing the optical conductivity, we can determine the dielectric function and refractive index of the silicene with thickness of Δ=0.4 nm.

$$\varepsilon = 1 + i\frac{\sigma(\omega)}{\varepsilon_0 \omega \Delta} \quad (7)$$

$$\varepsilon = \varepsilon' + i\varepsilon'' \quad (8)$$

$$N = \sqrt{\varepsilon} = n + \mathrm{i}k \quad (9)$$

$$n = \sqrt{\frac{\sqrt{\varepsilon' + \varepsilon''} + \varepsilon'}{2}} \quad (10)$$

$$k = \sqrt{\frac{\sqrt{\varepsilon' + \varepsilon''} - \varepsilon'}{2}} \quad (11)$$

3. Results and discussion

A. The effect of Fermi level (E_F) on the optical properties

In this section, we evaluate the effects of Fermi level E_F on silicon optical conductivity, $\sigma(\omega)$, and refractive index, $N(\omega)$. Fig. 4 shows the real and imaginary parts of the silicene optical conductivity in the THz regime at 300 K for different values of Fermi level from 0 to 1 eV. As E_F increases, the real part of $\sigma(\omega)$ shifts toward higher frequencies. Also, to 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 using E_F control.

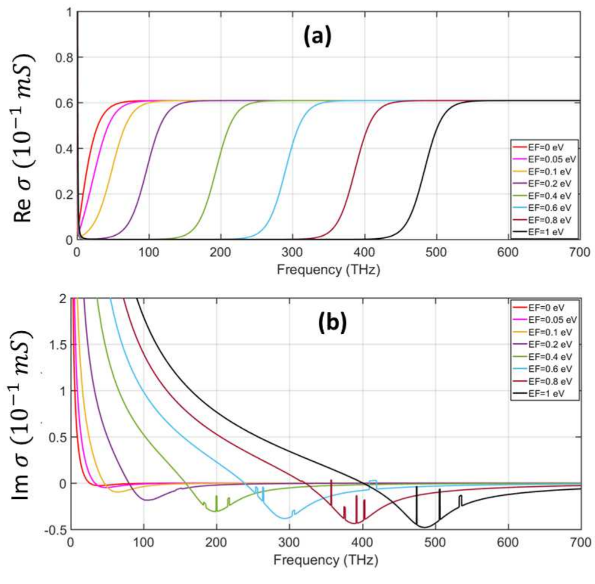

Fig 4. (a) Real and (b) imaginary parts of the silicene optical conductivity, $\sigma(\omega)$, at different Fermi levels.

Fig. 5 shows the real and imaginary parts of the silicene refractive index for different Fermi level values. As the Fermi level increases, the n amplitude decreases, and its peak shifts toward higher frequencies. The same effects are seen on the 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.

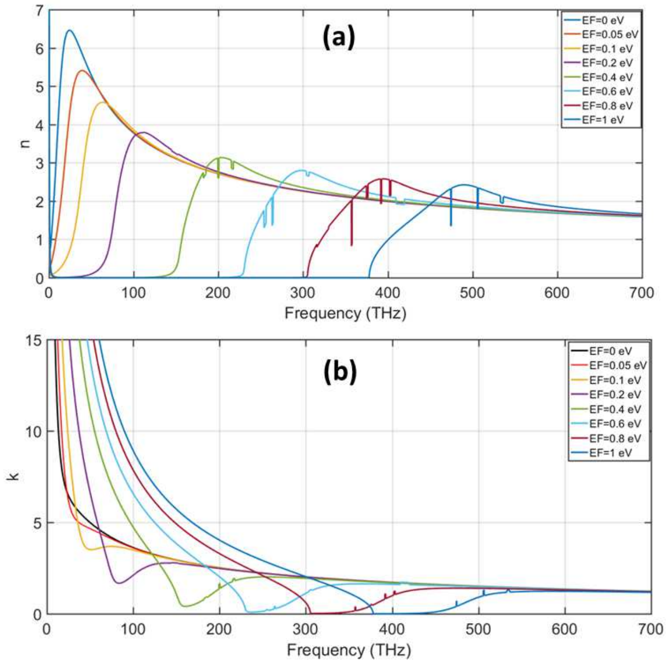

Fig. 5. (a) Real and (b) imaginary parts of the silicene refractive index vs. frequency at different Fermi levels.

B. The effect external electric field, E_z on optical properties

As mentioned, furthermore to E_F, the optical properties of silicene can be controlled by applying an electric field E_z. Fig. 6 shows the effect of the electric field E_z on the real and imaginary parts of the optical conductivity up to 2.5 eV at 300 K. The structure of silicene can withstand an external electric field E_z up to 2.6 eV, but will be unstable in higher fields [44]. For $E_z > 0.5$ eV, in addition to the shift, the amplitude of the real part increases. Moreover, increasing of E_z causes the amplitude and the range that imaginary part of $\sigma(\omega)$, has a negative value, increase. As a result, we have wider range for TE wave propagation. Compared to the effects of E_F, in here the range of negative values is larger.

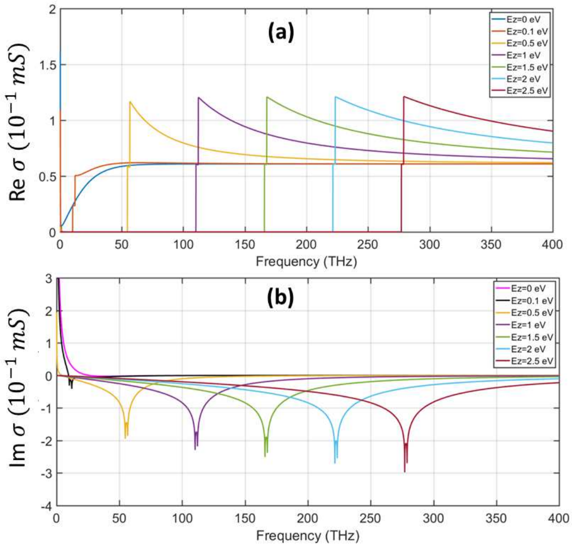

Fig. 6. (a) Real and (b) imaginary parts of the silicene optical conductivity, $\sigma(\omega)$, vs. frequency, at different external electric fields.

Fig. 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 get to the larger n amplitude.

We have the same effects on k, only the difference is that as E_z increases, the frequency range in which $k \approx 0$ expands.

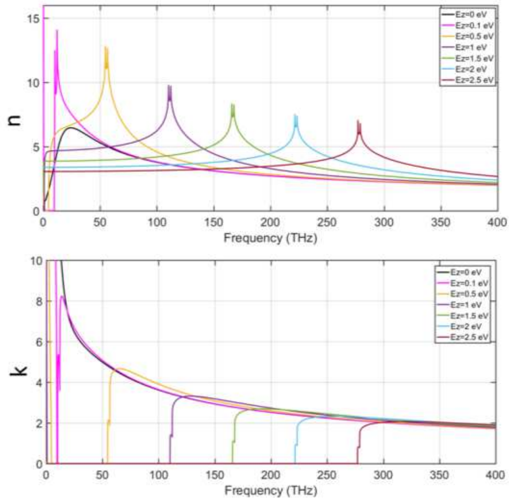

Fig. 7. (a) Real and (b) imaginary parts of the silicene refractive index vs. frequency at different external electric fields.

C. Temperature effects

Temperature can also affect the optical properties of the silicene. Fig. 8 shows the temperature variation effects on the silicene conductivity, $\sigma(\omega)$, for E_z=0.1 eV 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. Also at higher temperature, the amplitude of the conductivity peak is reduced. The thermal effects on the imaginary part of the optical conductivity are significant, too. As can be seen from the figure, by rising the temperature, the magnitude of negative values of imaginary part is reduced, so that at 400 K we have almost no negative value.

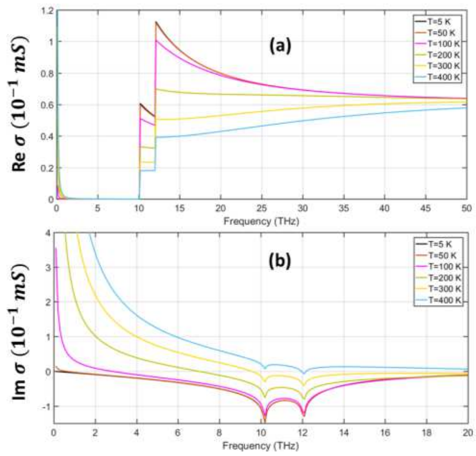

Fig. 8. (a) Real and (b) imaginary parts of silicene optical conductivity, $\sigma(\omega)$, vs. frequency at different temperatures.

The effect of temperature on the silicene refractive index is shown in Fig. 9. As the temperature rises, the real part amplitude of the refractive index decreases (Fig. 9(a)). Fig. 9(b) shows the effects of temperature on the imaginary part of the refractive index.

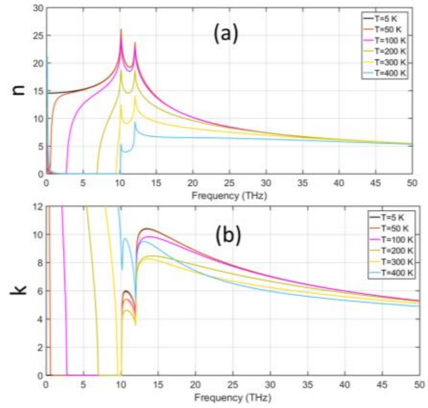

Fig. 9. (a) Real and (b) imaginary parts of the silicene refractive index vs. frequency at different temperatures.

D. Optical Properties at wavelength of 1550 nm

In this section, we present the effects of the Fermi level and the external electric field at room temperature and wavelength of 1550 nm. Fig. 10 shows the effect of Fermi energy variations at wavelengths of 1550 nm on the silicene optical conductivity. The real part of the silicene optical conductivity up to 300 meV is almost constant and equal to 0.06 mS, and at 500 meV this value becomes very negligible. The effect of 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 amount is almost zero. Also, as the Fermi level increases, the imaginary part of the silicene optical conductivity becomes negative, and in 400 meV, one can see the maximum negative amplitude. With more enhancement of the Fermi level, the quantity of the imaginary part changes from negative values to positive values. Fig. 11 shows the effects of the Fermi level on the silicene refractive index at wavelengths 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 rises further, the real part amplitude of the refractive index decreases and at higher than 500 meV almost becomes negligible. Also, around the 500 meV of Fermi level, the amplitude of the imaginary part of the silicene refractive index, reaches its lowest value, and with increasing the formal level, it will be increased.

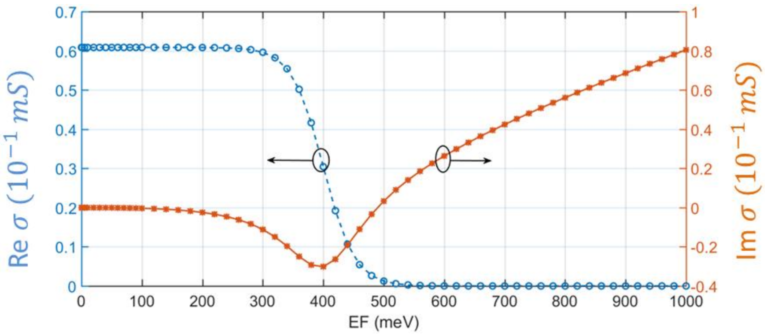

Fig. 10. Effect of Fermi Level variation on the real and imaginary parts of the silicene optical conductivity at the wavelength of 1550 nm.

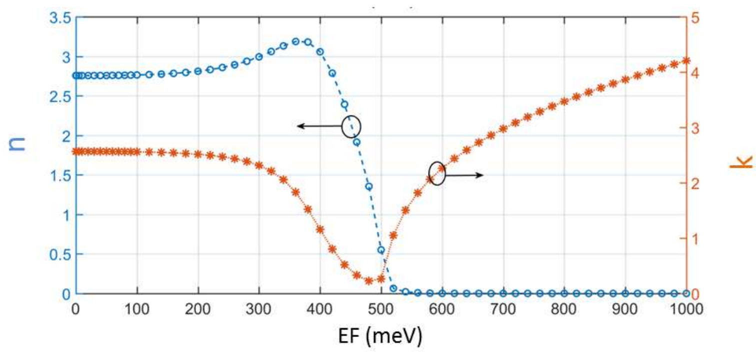

Fig. 11. Effect of Fermi Level variation on real and imaginary parts of silicene refractive index at the wavelength of 1550 nm

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

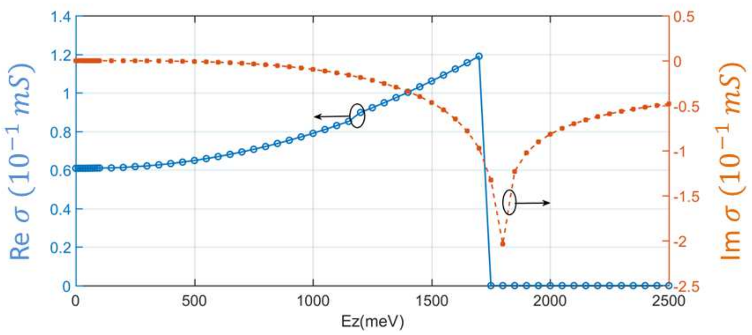

Fig. 12. Effect of external electric field on the silicene optical conductivity at wavelength of 1550 nm.

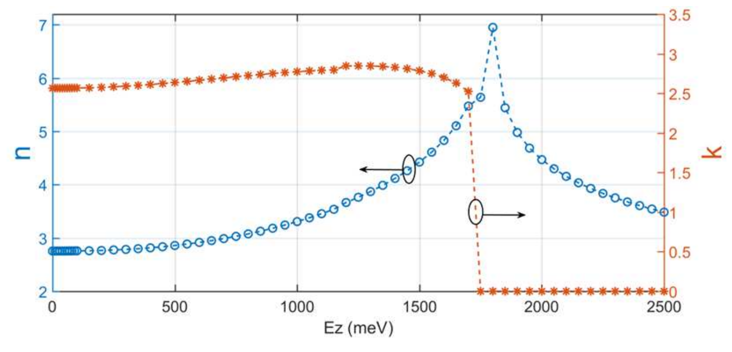

Fig. 13. Effect of external electric field on the silicene refractive index at wavelength of 1550 nm.

Conclusion

In this work, we examined the optical properties of silicene under such effects as 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 the external field of 0 eV and the temperature of 300 K. We also examined the effects of the external field in the range of 0 to 2.5 eV with the Fermi level of 0 eV and the 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, to further investigate the effects of Fermi level and external field on the optical conductivity and refractive index of silicene at the Wavelength of 1550 nm. The results showed that the effects of the external electric field were greater than the Fermi level on the optical conductivity and refractive index of silicene.

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Data will be available whenever a researcher requests access to the data.

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