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Tension effect on the absorbance of a graphene layer

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ABSTRACT
The effect of uniform planar tension on the absorbance of a graphene layer located between air and a semi-infinite dielectric medium has been investigated. The results show that the magnitude of the Van Hove peaks in the absorbance of the graphene depends on the tension direction, the strain modulus and the angle between the tension direction and the tangential electric field. While, the frequency location of the Van Hove peaks only depends on the tension direction and the strain modulus and is independent from the angle between the tension direction and the tangential electric field. When the tangential electric field is perpendicular to one of the vectors connecting a given carbon atom to its nearest neighbours, the related peak disappears. While, for the tangential electric field parallel to those vectors, the related peak acquires its largest value. Moreover, it is shown that the absorbance of the graphene layer at the low photon energies doesn’t noticeably depend on the tension direction, the strain modulus and the angle between the tension direction and the tangential electric field.

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1. Introduction
Graphene is a flat two-dimensional monolayer of carbon atoms arranged in a honeycomb crystal lattice that exfoliated from graphite in 2004 (1). Due to its unique thermal, mechanical, optical and electrical properties, graphene has attracted great interest (2–6). The reflectance, transmittance and absorbance of the graphene in the infrared and visible spectral range can be expressed in terms of the fine structure constant which is one of the remarkable optical properties of the graphene (6–9). Graphene has the potential to be used in photonic and optoelectronic devices such as photo-detectors, optical modulators, ultrafast lasers, filters, switches, beam splitters, polarizers, waveguides, touch screens displays, light-emitting diodes and solar cells (5, 6, 10, 11).

Recently, the strain effect on the device performance has been studied and the strain engineering has appeared in the graphene electronics (12, 13). The applied strain to a graphene layer (by compressing or stretching it out of the equilibrium) alters its band structure and may have important effects on the electronic and optical properties of the graphene. These effects depend on the strain modulus and the direction of the applied strain (13–16). The types of the uniform strain in the graphene are shear strain, the compressive uniaxial strain and the tensile uniaxial strain (tension) (16).

In this paper, the effect of a uniform planar tension on the absorption of a graphene layer has been interested. By applying the boundary conditions of the electromagnetic fields at the interface, the absorbance of the graphene can be calculated and expressed in terms of its optical conductivity (11). It is shown that the tension can affect the absorption of the graphene layer by altering the optical conductivity of the graphene. The paper is organized as follows. In Section 2, we introduce the system under consideration. Then the expressions for calculating the optical conductivity of the graphene are introduced and the effect of the tension on the optical conductivity is declared. In Section 3, the tension effect on the absorption of the graphene layer has been studied at different situations in which the graphene sheet strained along different directions. Finally, we summarize our results in Section 4.

2. Model and basic equations
We consider a graphene-based structure consisting of an infinitesimally thin graphene sheet, with the conductivity $\sigma$, which is located in the $z = 0$ plane between air and a semi-infinite nonmagnetic dielectric medium of relative dielectric permittivity $\varepsilon_d$, as shown schematically in Figure 1(a). Suppose that the electromagnetic wave is incident from air upon the graphene layer. By applying the boundary conditions of the electromagnetic fields at the graphene interface, the absorbance of the graphene layer for the TE (or $s$-polarized) and TM (or $p$-polarized) waves, are obtained as:
where $\varepsilon_0$ and $c$ are the vacuum permittivity and the speed of light in vacuum. $\alpha_1$ and $\alpha_2$ are the incident and the refracted angles respectively \((11)\), which satisfy Snell’s law \((\sin \alpha_1 = \sqrt{\varepsilon_0} \sin \alpha_2)\).

Here, we are interested to the effect of the uniform planar tension on the absorbance of the graphene layer. The graphene honeycomb lattice, its zigzag and armchair directions and the direction of the applied tension are shown in Figure 1(b). Here, the vectors connecting a given carbon atom to its nearest neighbours, have been denoted by $\delta_l$ \((l = 1, 2, 3)\). In unstrained graphene, these vectors are shown by $\delta^0_i$. As illustrated in Figure 1(c) and (d), the electric field of the TE-polarized wave \((E_t)\) is along the $y$ direction, and the electric field of the TM-polarized wave has a component along the $x$ direction \((E_p)\). The angle between the tension direction and the tangential electric field \((E_t\ or \ E_{p,x})\) has been denoted by $\phi$, in both polarizations. There are three zigzag directions in the graphene honeycomb lattice. Here, one of them is selected as the source zigzag direction. So, the tension direction has been located between the tangential electric field \((E_t\ or \ E_{p,x})\) and the source zigzag direction. The angle between the tension and the source zigzag direction has been denoted by $\theta$, in both polarizations.

The total optical conductivity of the graphene \((\sigma)\) is the sum of two contributions: the intraband conductivity \((\sigma_{\text{intra}})\) which corresponds to the intraband electron-phonon scattering processes and the interband conductivity \((\sigma_{\text{inter}})\) that originates from the direct interband electron transitions \((17)\). Expressions for the intraband conductivity and the real part of the interband conductivity have been derived using perturbation theory and are given by \((9, 18)\)

\[
\sigma_{\text{intra}}(\omega) = \frac{ie^2}{2\pi^2\hbar(\omega + i\Gamma)} \sum_{m=-\infty}^{\infty} \int_{BZ} \left| \frac{\partial E_m}{\partial k_\rho} \right|^2 \times \delta(E_m - \mu_c) d^2k, \tag{3}
\]

and

\[
\text{Re} \left( \sigma_{\text{inter}}(\omega) \right) = \int_{BZ} (f(E_-) - f(E_+)) \left| \frac{\partial \mathcal{H}}{\partial \rho} \right| \left| \frac{\partial \mathcal{H}}{\partial \rho} \right| \times \frac{e^2}{2\pi\hbar^2\omega} \delta(E_+ - E_- - \hbar\omega) d^2k \tag{4}
\]

Here, $\omega$, $e$, $\hbar$, $\Gamma$, $\mu_c$ and $k_\rho$ are the radiation frequency, the free electron charge, the reduced Planck constant, the phenomenological scattering rate, the chemical potential (Fermi level) and the Bloch wavevector component along the tangential electric field, respectively. $\mathcal{H}$ is the Hamiltonian matrix, $|c\rangle$ and $|v\rangle$ denote the conduction and valence bands eigenvectors, respectively. $E_+$ and $E_-$ are the conduction and valence bands energies, respectively. Here, the integrals are evaluated across the Brillouin zone. The Fermi–Dirac distribution is given by:

\[
f(\omega) = \left( 1 + \exp \left( \frac{E_\pm - \mu_c}{k_B T} \right) \right)^{-1}, \quad \tag{5}
\]

where $T$ is the temperature and $k_B$ is Boltzmann constant. The imaginary part of the interband conductivity can be calculated by using the Kramers–Kronig relation:

\[
\text{Im} \left( \sigma_{\text{inter}}(\omega) \right) = \frac{2\omega}{\pi} \int_{0}^{\infty} \frac{\text{Re} \left( \sigma_{\text{inter}}(\omega') \right)}{\omega^2 - \omega'^2} d\omega'. \tag{6}
\]

Since the applied tension deforms the graphene lattice, one can relate $\delta_l$ to $\delta^0_i$ as:

\[
\delta_l = \delta^0_l + T_{S} \delta^0_i, \quad \tag{7}
\]

where the strain tensor \((T_S)\) is given by \((14, 15)\)

\[
T_{S} = \zeta \left( \begin{array}{cc} \cos^2 \theta & - \eta \sin \theta \sin^2 \theta (1 + \eta) \sin \theta \cos \theta \\ (1 + \eta) \sin \theta \cos \theta & \sin^2 \theta - \eta \cos^2 \theta \end{array} \right). \tag{8}
\]

Here, $\zeta$ is the strain modulus and $\eta \approx 0.14$ is Poisson’s ratio \((19)\). By applying the nearest-neighbor tight-binding approximation, the Hamiltonian matrix for the strained graphene lattice and its conduction and valence bands energies are given as \((9, 15, 18)\):

\[
\mathcal{H} = \begin{pmatrix} 0 & -f_k \varepsilon \delta_k \\ -f^*_k \varepsilon \delta_k & 0 \end{pmatrix}, \quad \tag{9}
\]

\[
E_{\pm} = F_k + \sqrt{F_k^2 + \left( 1 - |g_k|^2 \right) |f_k|^2}, \quad \tag{10}
\]

with $f_k = \sum_{i=1}^{3} t_i e^{i \delta \hat{k} \cdot \hat{r}}$, $g_k = \sum_{i=1}^{3} s_i e^{i \delta \hat{k} \cdot \hat{r}}$, and $F_k = \text{Re} \left( g_k f_k^* \right)$. Here, $\hat{r}$ is the Bloch wavevector, $t_i = t_0 e^{-3.37(\delta \cdot a_0)}$ and $s_i = s_0 e^{(\delta \cdot a_0)^2}$ are the nearest-neighbour hopping and overlap parameters, respectively. $t_0 \approx 2.7 eV$, $s_0 \approx 0.07$ and $a_0 = 1.42 \AA$ is the equilibrium C–C distance in an unstained graphene sheet \((14, 15)\).

Since the applied tension deforms the graphene lattice and distorts the reciprocal lattice, the Hamiltonian, the conduction and valence bands energies are tension-dependent \((15)\). In what follow we investigate the effect of the applied tension on the absorbance of the graphene layer using Equations (1) and (2).
3. Results and discussion

Throughout this paper, $\mu_c = 0.2$ eV, $h\Gamma = 0.01$ eV, $T = 300K$, $\varepsilon_d = 2.25$ and $\alpha_1 = 30^\circ$ have been used. First of all, the absorbance of the strained graphene layer is plotted as a function of the photon energy ($h\nu$) for (a) the TE and (b) the TM waves in Figure 2. Here, it is assumed that $\zeta = 0.14$, $\varphi = 45^\circ$ with four different tension directions $\theta = 0^\circ$, $15^\circ$, $30^\circ$ and $45^\circ$. For comparison, the absorbance of an unstrained graphene layer ($\zeta = 0$) is plotted in Figure 2(c) for both TE and TM waves. As it is clear from Figure 2(a) and (b), the absorption of the graphene layer at the low photon energies ($h\nu < \mu_c$) doesn’t noticeably depend on the tension direction. Moreover, there are some peaks in the absorbance of the graphene layer at $h\nu > \mu_c$. The peaks are related to the Van Hove singularities at the saddle-points of the electronic band structure of the graphene layer (15). An unstrained graphene layer with $\delta_1 = \delta_2 = \delta_3 = a_0$ has three saddle-points in its electronic band structure which show themselves as a single peak in the absorbance spectrum at $h\nu \approx 2\mu_0$ (see Figure 2(c)). In the strained graphene layer along the zigzag ($\theta = 0^\circ$) or armchair ($\theta = 30^\circ$) directions, only two of the $\delta_1$, $\delta_2$ and $\delta_3$ are the same and the other one is different. Hence, in such a case, two peaks appear in the absorbance of the graphene layer. For the tension along the other directions, $\delta_1 \neq \delta_2 \neq \delta_3$. As a result, three peaks must be seen in the absorbance of the graphene layer. However, as it is seen from Figure 2(a) and (b), there are two peaks in the absorbance of the graphene layer at $\theta = 15^\circ$. Here, $\varphi$ is considered to be $45^\circ$, so we have $\theta + \varphi = 60^\circ$. In this case, the tangential electric field lies along the zigzag direction (see Figure 1(c) and (d)) and thus it will be perpendicular to one of the $\tilde{\delta}_1$, $\tilde{\delta}_2$ or $\tilde{\delta}_3$. Hence, the tangential electric field can’t induce electric dipole between the two neighbour atoms in the normal direction. Consequently, the related peak disappears. Figure 2(a) and (b) reveal that the locations of the absorbance peaks for the TE and the TM waves are identical. However, their peak values are slightly different. To show this, the relative difference between $A_s$ and $A_p$ are plotted as a function of the photon energy in Figure 2(d). As it is clear from the figure, in the most frequencies, $A_s$ is about 8.5 we will study only $A_s$.

In Figure 3, the absorbance $A_s$ is plotted in the plane of the photon energy and the tension direction with $\zeta = 0.14$ and $\varphi = 45^\circ$. As the figure reveals, there are generally three peaks in the absorbance $A_s$ which their locations and magnitudes strongly depend on the tension direction. The strong peak is blue shifted from $h\nu \approx 1.89$ eV to $h\nu \approx 5.8$ eV by increasing $\theta$ from $\theta = 0^\circ$ to $\theta = 60^\circ$. The second peak which is a relatively weak peak is red shifted from $h\nu \approx 5.8$ eV to $h\nu \approx 1.89$ eV by increasing

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**Figure 1.** Geometry of the problem: (a) An infinitesimally thin graphene sheet located in the $z = 0$ plane between air and a semi-infinite dielectric medium. (b) The graphene honeycomb lattice, its zigzag and armchair directions and the tension direction. (c) The angle $\varphi$ between the tension direction and the tangential electric field and the angle $\theta$ between the tension direction and the source zigzag direction in the case of the TE polarization. (d) Same as figure (c) for the case of the TM polarization.
Figure 2. The absorbance of the strained graphene layer as a function of photon energy ($h\nu$) for (a) the TE and (b) the TM waves, respectively; (c) the absorbance of the unstrained graphene ($\zeta = 0$) as a function of $h\nu$; (d) the relative difference between $A_s$ and $A_p$ as a function of $h\nu$ in the case of the strained graphene layer. Here, $\varphi = 45^\circ$ and $\zeta = 0.14$ for the cases of the strained graphene layer.

Figure 3. The absorbance $A_s$ in the plane of $(h\nu, \theta)$. Here, $\zeta = 0.14$ and $\varphi = 45^\circ$.

Now, we want to investigate the effect of the strain modulus on the absorbance of the graphene layer for the TE waves. To do this, the absorbance $A_s$ of the strained graphene layer is plotted in Figure 4 as a function of the photon energy ($h\nu$) at (a) $\theta = 0^\circ$, (b) $\theta = 15^\circ$, (c) $\theta = 30^\circ$, and (d) $\theta = 45^\circ$. Here, four different values are considered for the strain modulus i.e. $\zeta = 0$, 0.07, 0.14 and 0.21 with $\varphi = 45^\circ$. As expected, the absorbance of the graphene layer at the low photon energies ($h\nu < \mu_c$) doesn’t noticeably depend on the strain modulus. Figure 4(a)–(c) reveal that the absorbance $A_s$ of the strained graphene layer contains two peaks around $h\nu \approx 2\mu_c$ (the location of the absorbance peak of the unstrained graphene). The first peak is red shifted and the second one is blue shifted by increasing the strain modulus. In the case of $\theta = 45^\circ$, the absorbance $A_s$ of the strained graphene layer shows three peaks (see Figure 4(d)). Like as the previous cases, the first peak is red shifted and the third one is blue shifted by increasing the strain modulus. However, the second peak which is located at $h\nu < 2\mu_c$ is red shifted by increasing the strain modulus.

Finally, we want to investigate the effect of $\varphi$ (the angle between the tension direction and the tangential electric field) on the absorbance of the graphene layer. To do this, the absorbance $A_s$ of the strained graphene is plotted in the plane of the photon energy ($h\nu$) and $\varphi$ in Figure 5 at (a) $\theta = 0^\circ$ and (b) $\theta = 15^\circ$ with $\zeta = 0.14$. The figure reveals that the absorbance of the graphene layer at the low photon energies ($h\nu < \mu_c$) doesn’t noticeably depend on the angle between the tension direction and the tangential electric field. Depending on the values of $\varphi$ and $\theta$, the absorbance of the strained graphene layer may contains up to three peaks. In the case of $\theta = 0^\circ$, the absorbance of the strained graphene layer has two peaks at $h\nu \approx 1.89$ eV and $h\nu \approx 5.8$ eV (see Figure 5(a)). The low energy peak is related to $\delta_2$ and the high energy peak is related to both of $\delta_1$ and $\delta_3$ (because $\delta_1 = \delta_3$). As it is seen from Figure 1(b) and (c), the tangential electric field lies along the zigzag direction and is perpendicular to $\delta_2$ at $\theta = 0^\circ$ with $\varphi = 0^\circ$ or $\varphi = 180^\circ$ which causes the first peak to vanish (see Figure 5(a)). At the same time,
Figure 4. The absorbance $A_s$ of the strained graphene layer as a function of the photon energy ($h\nu$) at (a) $\theta = 0^\circ$, (b) $\theta = 15^\circ$, (c) $\theta = 30^\circ$, and (d) $\theta = 45^\circ$ for four different values of the strain modulus $\zeta = 0, 0.07, 0.14$ and 0.21 with $\phi = 45^\circ$.

Figure 5. The absorbance $A_s$ of the strained graphene in the plane of $(h\nu, \phi)$ at (a) $\theta = 0^\circ$ and (b) $\theta = 15^\circ$ with $\zeta = 0.14$.

4. Conclusion

The effect of a uniform planar tension on the absorbance of a graphene layer located between air and a semi-infinite dielectric medium has been investigated in different situations. By applying the tension along different directions the Van Hove peak in the absorbance of the unstrained graphene may be split into two or three. The frequency locations and the magnitudes of the peaks strongly depend on the tension direction and the strain modulus. The frequency interval between the peaks depend on the strain modulus and increases by increasing it. However, the frequency location of the Van Hove peaks is independent from the angle between the tension direction and the tangential electric field. Whilst, the value of Van Hove peaks depends on the angle between the tension direction and the tangential electric field. When the tangential electric field is perpendicular to one of the vectors that connecting a given carbon atom to its nearest neighbours, the related peak disappears. Nevertheless, if the tangential electric field lies along one of the $\delta_1$, $\delta_2$ or $\delta_3$. This situation is correspond to the case of $\phi \approx 15^\circ, 75^\circ$ or $135^\circ$ with $\theta = 15^\circ$ as shown in Figure 5(b).
the tangential electric field. Our results may be useful in designing the various graphene-based optoelectronic devices.

**Disclosure statement**

No potential conflict of interest was reported by the authors.

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**References**


