Theory of dielectric loss in Graphene-on-substrate: A tight-binding model study

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Abstract. Graphene-on-substrate exhibits interesting dielectric behaviour due to screening of coulomb interaction induced by many body effects. In this communication we attempt to study the dielectric loss property of graphene within tight-binding model approach. The Hamiltonian consisting of electron hopping up to third-nearest-neighbour’s with impurities in two in equivalent sub-lattices. The graphene-on-substrate raises the energy $+\Delta$ at one sub lattice and reduces energy $-\Delta$ at other sub lattice. Further we introduced coulomb interaction between $\pi$ - electrons at the two sub lattices separately with the same effective coulomb interaction. We calculate polarization function $\Pi(q, \omega)$ which is a two particle Green's function arising due to charge-charge correlation by using Zubarev's Green's function technique. Finally we calculate dielectric function of graphene i.e. $\epsilon(q, \omega) = 1 + \Pi(q, \omega)$ at arbitrary wave vector $q$ and frequency $\omega$. The dielectric loss in graphene calculated from the imaginary part of dielectric function which is a measure of absorption spectrum. Only a few Fragmentary theoretical attempts have been made to utilize the full frequency and wave vector dependent dielectric function. We compute numerically the frequency dependent dielectric loss function for 100x100 momentum grid points. We observe a low energy Plasmon resonance peak and a high energy flat peak arising due to absorption of optical energy at substrate induced gap. With increase of small Plasmon wave vector, both low and high energy peaks approach each other. The dielectric loss at low energies exhibits a parabolic curve, but it exhibit a clear peak on introduction of higher order electron hopping’s. The Coulomb interaction suppresses induced gap in graphene and decreases the optical energy absorption spectra. The increase of substrate induced gap shifts the high energy flat peak to higher energies and enhances the dielectric loss throughout the frequency range. Finally the effect of doping on dielectric loss is investigated and compared with the experimental results.

Keywords: Dielectric loss , coulomb interaction, dielectric polarization

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1. Introduction

The graphene with a honey-comb lattice structure exhibits a gap less semiconductor with linear dispersion relation in electron momentum in the vicinity of the two in equivalent corners of the hexagonal brillouin zone [1]. Due to the lack of band gap in graphene, the pristine graphene cannot be used in spintronic device applications. Therefore, intense attempts have been made both experimentally and theoretically to induce a band gap near Dirac point by several techniques like introducing impurities, ad-atoms, defects, different substrates, Coulomb correlation etc. [2]. The optical spectroscopy has proven to be an excellent probe to study band gap opening in graphene system. When infrared radiation is incident on graphene, the \( \pi \)-electron Plasmon vibration sets in graphene with a wave vector dependent Plasmon frequency. The optical frequency response of graphene leads to the dielectric function. There are a very few theoretical studies on frequency and temperature dependent dielectric function taking into account the electronic dispersion throughout the brillouin [3,4]. Hwang et. al. [5] have reported theoretical study of dielectric constant and plasmon dispersion in two dimensions. More recently Abergel have reported theoretical study of dielectric constant and plasmon dispersion in two dimensions. In this report, we have considered a tight-binding model containing electron and hole doping effects, substrate induced gap as well as on-site Coulomb interaction at two sub-lattices of graphene. We attempt here to calculate the dielectric response function and hence the dielectric loss from its imaginary part graphene system [6].

2. Theoretical Model

The tight-binding model Hamiltonian for honey-comb lattice of graphene is written as

\[
H_1 = \sum_{k,\sigma} (\epsilon_a a_{k,\sigma}^\dagger a_{k,\sigma} + \epsilon_b b_{k,\sigma}^\dagger b_{k,\sigma}) + \sum_{k,\sigma} V (x_a a_{k,\sigma}^\dagger a_{k,\sigma} + x_b b_{k,\sigma}^\dagger b_{k,\sigma}) + \sum_{k,\sigma} \Delta (a_{k,\sigma}^\dagger a_{k,\sigma} - b_{k,\sigma}^\dagger b_{k,\sigma}) - \\
\sum_{\beta=1,3} \sum_{k,\sigma} t_\beta (y_\beta(k) a_{k,\sigma}^\dagger b_{k,\sigma} + y_\beta^*(k) b_{k,\sigma} a_{k,\sigma}) + U \sum_i [n_{i,\uparrow} n_{i,\downarrow} + n_{i,\downarrow} n_{i,\uparrow}^\dagger] + \text{term} - \text{term} \quad (1)
\]

The first term in the Hamiltonian given in equation (1) describes the on-site electron hoppings at A and B sub lattices of graphene with site energies \( \epsilon_a \) and \( \epsilon_b \). The second term represents the doping effect at both the sub lattices with interaction potential \( V \) and concentrations \( x_a \) and \( x_b \). The third term describes the interaction for graphene-on-substrates where A (B) sub lattice is raised (reduces) with energy \(+\Delta \) (\( -\Delta \)). According to our earlier reports [7-14], the fourth term represents the tight-binding Hamiltonians with electron hoppings up to third nearest -neighbours and \( t_\beta \) and \( y_\beta(k) \) represent hopping parameters and band dispersion for \( \beta = 1, 2, 3 \). Finally the last term in the Hamiltonian describes on-site Coulomb repulsive interactions for both sub lattices with electron densities \( n_{i,\sigma} = a_{i,\sigma}^\dagger a_{i,\sigma} \) and \( n_{i,\sigma}^\dagger = b_{i,\sigma}^\dagger b_{i,\sigma} \).

3. Calculation of dielectric loss function

The frequency (\( \omega \)) and wave vector (\( q \)) dependent dielectric function is written as \( \epsilon(q, \omega) = 1 + \Pi(q, \omega) \), where the polarization function which describes the charge-charge correlation is written as \( \Pi(q, \omega) = \)
and charge function is defined as \( \rho(q, t) = \sum_{k, \sigma} (a_{k+q, \sigma}^\dagger a_{k, \sigma} + b_{k+q, \sigma}^\dagger b_{k, \sigma}) \). The polarization function is a two particle Green’s function involving four other functions which are calculated by using the total electronic Hamiltonian given in equation (1) employing Zubarev’s techniques. The four coupled Green’s are solved and finally the frequency and wave vector dependent polarization function \( \Pi(q, \omega) \) is calculated. The dielectric loss is directly proportional to imaginary part of the polarization function. The dielectric loss coefficient is computed numerically and is plotted by varying different physical parameters of the graphene system like impurity concentration, substrate induced gap, Coulomb-correlation and Plasmon wave vector.

4. Result and Discussion

In order to investigate the effect of Coulomb interaction in \( \Pi(q, \omega) \), we evaluate numerically and self-consistently the electron occupancies at A and B sub lattices for up and down spin orientations. Finally dielectric loss coefficient is computed numerically by taking \( 100 \times 100 \) grid points for the electron momentum taking different physical parameters of the systems. The plots are shown in figures 1 to 3. The physical parameters involved in the calculation are made dimensionless with respect to nearest-neighbour-hopping integral \( (t_1) \). The parameters are \( \tilde{t}_1 = -1 \), \( \tilde{t}_2 = \frac{t_2}{t_1} \), \( \tilde{t}_3 = \frac{t_3}{t_1} \), impurity potential \( \nu = \frac{V}{2} \), Coulomb potential \( \nu = \frac{U}{t_1} \), temperature \( t = \frac{k_B T}{t_1} \), applied external frequency \( c_1 = \frac{\omega}{t_1} \) and substrate induced gap \( d_1 = \frac{\Delta}{t_1} \), plasmon momentum transfer energy \( q_x = \frac{v_F q}{t_1} \), where \( v_F \) and \( q \) are respectively the velocity of electrons at Fermi level and plasmon wave vector.

The imaginary part of dielectric function describes the dielectric loss i.e. \( \text{Im}\varepsilon(q, \omega) = \text{Im}\chi(q, \omega) \) in graphene in present calculation. The dielectric loss is plotted vs. optical energies for small plasmon wave vectors, \( \varepsilon = 0.01, 0.02, 0.03 \) in the long wave limit. The dielectric loss exhibits a divergent peak \( p_1 \) at energy \( c_1 \rightarrow 0 \). This singular structure arises from the characteristics of the inter band excitation energy \( \Delta E = \omega_x (k_x + q_x, k_y + q_y) , \Delta y (k_x, k_y) \) in the wave vector space. \( \Delta E \) near the peak \( p_1 \) points to isotropic and linear at very small \( q_x \) and \( q_y \). Fig. 1 shows that the peak \( p_1 \) increases with increase of wave vector and shifts to higher energies. The \( \pi \)-band model calculation here is used to study the singular structure. We observe here another flat singular structure \( p_2 \) at higher energy arising due to substrate induced gap \( d_1 \). If results from the excitations of the middle points of a step like structure. The position of the peak remains unchanged with wave vector.
**FIGURE 1.** The plot of dielectric loss vs. energy \( (c_1) \) for different values of Plasmon wave vector \( q_x \) for given substrate induced gap \( d_1 = 0.04 \) for Coulomb potential \( u = 2.2 \), damping factor \( e_1 = 0.001 \) at temperature \( t = 0.025 \).

**FIGURE 2.** The plot of dielectric loss vs. energy \( (c_1) \) for different substrate induced gap \( d_1 = 0.02, 0.03, 0.04, 0.05 \) for fixed Coulomb potential \( u = 2.2 \), damping factor \( e_1 = 0.001 \) and temperature \( t = 0.025 \) for plasmon wave vector \( q_x = 0.03 \).

Figure 2. shows the effect of substrate on the dielectric loss. For a given substrate induced gap \( d_1 = 0.02 \), we observe a Plasmon momentum transfer energy peak \( (p1) \) at lower energy and a high energy excitation peak \( (p2) \) arising due to the substrate induced gap at energy \( c_1 \sim 0.22 \). The dielectric loss remains nearly uniform at
higher energies. When substrate induced gap increases from \( d_1 = 0.02 \) to 0.05, the high energy excitation peak becomes flat and moves to higher energies (see the inset of fig. 2). Again the dielectric loss remains constant at higher energies. It is noted further that the dielectric loss or absorption of optical energy increases with increase of the magnitude of the substrate induced gap. The experimental measurements of graphene on different substrates exhibit gaps of energy 100 meV for graphene on BN [15], 200 meV for gold on ruthenium [16] and 250 meV for graphene on SiC [17].

![Image](image.png)

**FIGURE 3.** The plot of dielectric loss vs. energy (c1) for different Coulomb potential \( u = 1.7, 2.0, 2.2, 2.5 \), fixed Substrate induced gap \( d_1 = 0.04 \) at temperature \( t = 0.025 \) plasmon wave vector \( q_x = 0.03 \).

The electron-electron interaction is absent in pristine graphene. However, electron–electron interaction plays an important role for graphene on substrates for different impurity concentration. In figure 3, we show the effect of Coulomb interaction i.e. \( u = 1.7 \) to 2.5 on the dielectric loss of graphene on a given substrate. The dielectric loss or optical energy absorption becomes less and less with increase of Coulomb interaction energy \( (u) \). It is noted that the low energy plasmon momentum excitation peak \( (p_1) \) remains unaltered at its position while the high energy substrate induced gap excitation peak \( (p_2) \) is suppressed (see inset of fig. 3) with increase of Coulomb energy. However the dielectric loss remains nearly constant at higher energies.

### 5. Conclusion

We have calculated the dielectric loss or optical energy absorption co-efficient from the imaginary part of the dielectric function for graphene-on-substrate by tight-binding approach using Green’s function technique. We have studied the evolution of low energy Plasmon momentum transfer energy excitation peak and substrate induced gap excitation peak by varying Plasmon momentum, substrate induced gap and Coulomb energy.
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