



## اثرات فونون سطحی زیر لایه بر جذب پلاسمونی گرافن

شراره جلالوندی<sup>۱</sup>، محمد کاظم مروج فرشی<sup>۱</sup> و سارا درباری<sup>۱</sup>

<sup>۱</sup> دانشکده مهندسی برق و کامپیوتر، دانشگاه تربیت مدرس، تهران، ایران

چکیده- در مقاله‌ی پیش رو روش جدیدی ارائه داده‌ایم که با استفاده از آن می‌توان تأثیر زیر لایه بر جذب پلاسمونی در گرافن را با ترکیب دو روش تقریب فاز تصادفی و معادلات انتگرالی مشاهده کرد. زیر لایه‌ی قطبی  $\text{SiO}_2$  و غیرقطبی DLC برای بررسی تغییرات جذب پلاسمونی در گستره‌ی میان-مادون قرمز در نانونوارهای گرافنی انتخاب شده‌اند. برهمکنش میان پلاسمون‌های برانگیخته شده در سطح گرافن و فونون‌های زیر لایه‌ی قطبی تغییر چشمگیری در پاسخ ساختار ایجاد می‌کند و در نتیجه تأثیر بر روی جذب پلاسمونی نیز چشمگیر خواهد بود. در اینجا، ابتدا با استفاده از تقریب فاز تصادفی تابع دی‌الکتریک گرافن را بدست می‌آوریم. آشکارا است که در حضور فونون، تابع دی‌الکتریک نسبت به زمانی که فونون حضور ندارد متفاوت است. پس از آن با مدل کردن گرافن با تابع دی‌الکتریک مناسبه شده و استفاده از روش معادلات انتگرالی جذب پلاسمونی را می‌یابیم. مطالعات ما راه را برای ساختارهای پلاسمونی مانند مدولاتورها، موجبرها و آشکارسازها و نحوه‌ی استفاده از زیر لایه‌ها روشن می‌کند.

کلید واژه- فونون، گرافن، جذب پلاسمونی، تقریب فاز تصادفی، روش معادلات انتگرالی.

## Effects of Substrate Phonons on the Graphene Plasmonic Absorption

Sharareh Jalalvandi<sup>1</sup>, Mohammad Kazem Moravvej Farshi<sup>2</sup>, Sara Darbari<sup>3</sup>

<sup>1,2,3</sup>Nano-Plasmo Photonics Research Group, Tarbiat Modares University, Tehran.

<sup>1</sup>[sharareh.jalalvandi@modares.ac.ir](mailto:sharareh.jalalvandi@modares.ac.ir), <sup>2</sup>[moravvej@modares.ac.ir](mailto:moravvej@modares.ac.ir), <sup>3</sup>[s.darbari@modares.ac.ir](mailto:s.darbari@modares.ac.ir).

**Abstract-** We propose a new method to show the effect of the substrate phonons on the plasmonic absorption in graphene nanoribbons. In doing so, first, we have used a random phase approximation method to compare the dielectric functions of the graphene layers patterned on a polar  $\text{SiO}_2$  and a nonpolar like diamond-like-carbon (DLC) substrates. Then, using the employing dielectric functions together with the integral equation method, we have compared the corresponding plasmonic absorptions in the mid-infrared wavelengths. The comparison has revealed the  $\text{SiO}_2$  surface phonons strongly interact with the graphene surface plasmons (SPs) at the wavelengths  $\lambda = 8.56$  and  $12.4 \mu\text{m}$ , modifying the related dielectric function and hence the plasmonic absorption significantly, as compared to that of the structured graphene on the nonpolar substrate. This study paves the way for designing graphene based plasmonic devices such as modulators, waveguides, and detectors.

**Keywords-** Phonon, Graphene, Plasmonic Absorption, Random Phase Approximation, Integral Equation Method.

## 1. Introduction

Graphene surface plasmons (SPs) have attracted great attention because of their long propagation length and confinement in very small volumes besides the graphene tunability, as compared to SPs in metals. Patterning a graphene sheet into nano/microstructures such as ribbons, disks, rings, or dots can provide the condition for conserving the incident light wavevector while exciting the graphene SPs [1]. The pattern geometry, doping level, and the substrate material define the SPs resonance frequency at which the plasmonic absorption peaks [2].

Moreover, vibrations of the electrically positive and negative atoms on the surface of polar substrates such as SiO<sub>2</sub> are quantized in the surface optical phonons, inducing an electric field that damps exponentially away from the surface. When the resonance frequency of SPs excited in structured graphene patterned on a polar substrate coincides with that of the substrate surface phonons, their electric fields strongly interact, resulting in the hybrid plasmon-phonon modes [2]. Conversely, a nonpolar substrate such as diamond-like-carbon (DLC) has no surface optical phonons to interact with the overlying graphene SPs. A SiO<sub>2</sub> substrate has two surface phonons at the mid-infrared wavelengths of 8.56 and 12.4  $\mu\text{m}$ , resulting in three hybrid plasmon-phonon modes in the overlying structured graphene [3]. For frequencies far below and far above the given frequencies, the hybrid modes approach to the plasmonic modes. Conversely, close to either of the two given wavelengths, the phonon modes become dominant.

A few research works have investigated the impact of the substrate surface phonons on the graphene plasmon modes [4-6], to dates, creating the hybrid plasmon-phonon modes. Nonetheless, this phenomenon deserves further theoretical investigations.

Hence, in this work, we devoted our efforts to describe the effect of phonons-plasmons coupling on the plasmonic absorption in arrays of graphene

nanoribbons, employing the random phase approximation (RPA) together with the integral equation method (IEM), for the first time.

## 2. Methods

To achieve our aims, first, we have used RPA for obtaining the dielectric function two arrays of graphene nanoribbons; one formed on a SiO<sub>2</sub> and the other on a DLC substrate. Then we used these dielectric functions and IEM to evaluate the plasmonic absorption in the structured graphene.

### 2.1 RPA and Dielectric function

In many-particle physics, the plasmon response of the electron gas begins with finding the dielectric function. To this aim, a common useful model is RPA. In this model, the electrons respond to a total potential,  $V_{\text{tot}}$ , which is the sum of the external potential,  $V_{\text{ext}}$ , and the screening potential,  $V_{\text{scr}}$ . Once  $V_{\text{tot}}$  is found, the dielectric function can be obtained from

$$\epsilon_{\text{RPA}}(q, \omega) = \frac{V_{\text{ext}}(q)}{V_{\text{tot}}(q, \omega)}, \quad (1)$$

where  $\epsilon_{\text{RPA}}$  is the RPA expansion of the dielectric function. To find  $V_{\text{tot}}$ , Feynman diagrams are useful. In many-particle systems with only electrons are involved, Feynman diagram looks like to Fig. 1, in which  $V_c(q) = e^2/2q\epsilon_0$  and  $\Pi_0$  are the Coulomb interact between two electrons and polarizability, respectively. It shows that the total potential consists of two parts, one is the interaction between two electrons and the other is the interaction between two electrons mediated by the other electrons. After some algebra we find

$$V_{\text{tot}}(q, \omega) = \frac{V_c(q)}{1 - V_c(q)\Pi_0(q, \omega)}. \quad (2)$$

For graphene we have

The diagram illustrates the total potential  $V_{\text{tot}}$  as the sum of two terms. The first term is the direct Coulomb potential  $V_c$ , represented by a wavy line. The second term is a screened potential, represented by a wavy line  $V_c$  followed by a loop containing the polarizability  $\Pi$ , which is then followed by another wavy line  $V_c$ . The entire second term is enclosed in a red oval. The final result is labeled  $V_{\text{eff}}$ .

Fig. 1: Feynman diagram for a many-particle system containing only electrons.

$$\Pi_0(q, \omega) \approx \frac{E_f q^2}{\pi \hbar^2 (\omega + i/\tau_e)^2}, \quad (3)$$

where  $E_f$  is Fermi energy,  $\hbar$  is reduced Planck's constant and  $\tau_e$  is the electron lifetime. It is obvious from Eq. (1) and Eq. (2) that the dielectric function in RPA can be written as

$$\varepsilon_{\text{RPA}}(q, \omega) = 1 - V_c(q) \Pi_0(q, \omega). \quad (4)$$

In a similar way, for systems with electrons and phonons, Feynman diagram can be sketched as shown in Fig. 2. Here, the dielectric function is

$$\varepsilon(q, \omega) = 1 - [V_c(q) + V_{ph}(q, \omega)] \Pi_0(q, \omega), \quad (5)$$

where  $V_{ph}(q, \omega)$  is the interaction between electrons mediated by phonons [7].

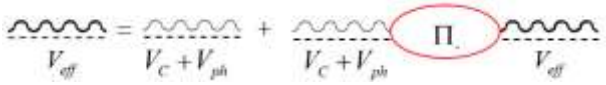


Fig. 2: Feynman diagram for a many-particle system containing electrons and phonons.

From electromagnetic, we know that the plasmon modes are obtained from the zeros of the dielectric function [8]. Graphene carriers can be considered as a 2D electron gas, so the dielectric functions of graphene, on nonpolar and polar substrates, is Eq. (4) and Eq. (5), respectively. Now, we can define plasmon modes for graphene substrates such as DLC and SiO<sub>2</sub> by equating them to zero, as shown in Fig. 3 when the Fermi level is 0.4 eV. As we mentioned, SiO<sub>2</sub> has two optical phonon frequencies in the mid-infrared range that changes the plasmon mode into three hybrid plasmon-phonon modes.

## 2.2. IEM and Plasmonic Absorption

To be able to use IEM for graphene nanoribbons on different substrates, we must first define Green's function for arrays of 1-D periodic ribbons. From

Green's function of line sources in a periodic grid, we find Green's function for periodic ribbons as

$$G_p(x, z | x') = \sum_{m=-\infty}^{\infty} \frac{e^{-jk_{zm}|z|}}{j2dk_{zm}} e^{jk_{xm}(x-x')}, \quad (6)$$

where  $G_p$  is the periodic Green's function,  $d$  is the periodicity,  $k_{xm} = k_x^i + \frac{2m\pi}{d}$ , and  $k_{zm}$  is defined as

$$k_{zm} = \begin{cases} \sqrt{k_0^2 - k_{xm}^2 - k_y^{i2}} & k_0^2 \geq k_{xm}^2 + k_y^{i2} \\ -j\sqrt{k_{xm}^2 + k_y^{i2} - k_0^2} & k_0^2 \leq k_{xm}^2 + k_y^{i2} \end{cases}, \quad (7)$$

where  $k_0$ ,  $k_x^i$ ,  $k_y^i$  are the incident wave vector in free space, along x and y, respectively [9]. Next, we must define the integral equations that we solve with this Green's function, Eq. (6). One way to model ultrathin periodic structures is an equivalent sheet model in which we have following boundary conditions,

$$\begin{aligned} \hat{n} \times [\mathbf{E}^+ - \mathbf{E}^-] &= 0, \\ \hat{n} \times [\mathbf{E}^+ + \mathbf{E}^-] &= 2R\hat{n} \times \hat{n} \times [\mathbf{H}^+ - \mathbf{H}^-], \end{aligned} \quad (8)$$

$R$  is the impedance of the graphene sheet,  $E^\pm$  and  $H^\pm$  are the electric and magnetic fields at just above and below of the sheet and  $\hat{n}$  is the unit normal in the + direction. It is known that reversing the conductivity, gives us  $R$ . For graphene, when plasmon is propagating we have,

$$\sigma(q, \omega) \approx \frac{i2\omega\varepsilon\varepsilon_0}{q}, \quad (9)$$

where  $\sigma$ ,  $\varepsilon$ , and  $\varepsilon_0$  are the conductivity, the dielectric function of graphene and free space permittivity, respectively.

As we mentioned recently, the dielectric function of graphene on polar and nonpolar substrates are obtained from Eq. (4) and Eq. (5), respectively. We use them in Eq. (9) to model the conductivity of graphene and then find sheet impedance on different substrates. After that, by putting  $R$  in Eq. (8), and following the IEM method procedures with defined

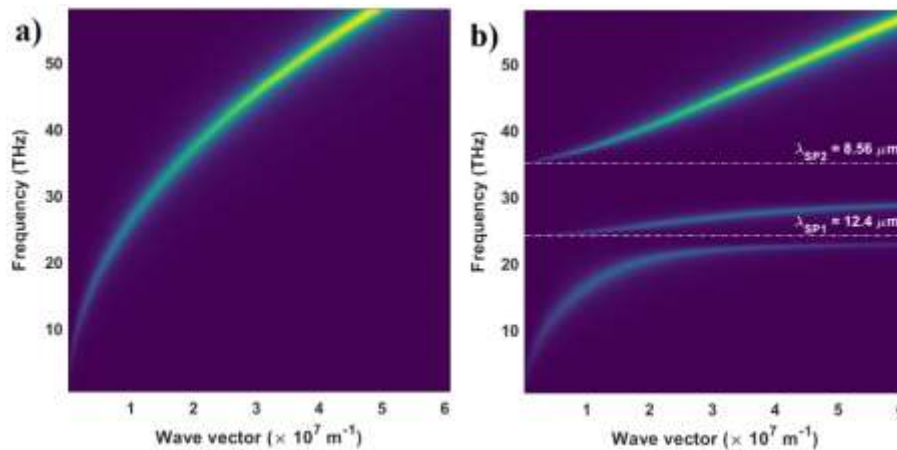


Fig 3. Plasmon dispersion for an array of graphene nanoribbons on a (a) DLC substrate with no optical phonons; and (b) SiO<sub>2</sub> substrate with two surface phonons.

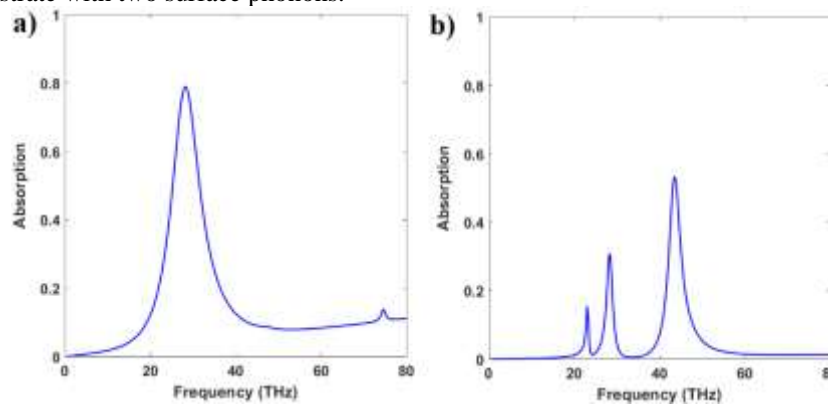


Fig 4. Plasmonic absorption for an array of graphene nanoribbons on a (a) DLC substrate with no optical phonons; and (b) SiO<sub>2</sub> substrate with two surface phonons.

Green's function, Eq. (6), we find plasmonic absorption, as shown in Fig. 4. Here, the width of nanoribbons is chosen to excite plasmon in the CO<sub>2</sub> laser frequency, ~29 THz.

### 3. Conclusion

We have combined two well-known techniques — i.e., the random phase approximation and integral equation method, — to show how a polar substrate can affect the plasmonic absorption in an overlaying array of graphene nanoribbons. The simulation results have demonstrated that the surface phonons on the SiO<sub>2</sub> substrate modify the graphene plasmonic absorption remarkably about the frequencies of the surface optical phonons in SiO<sub>2</sub> ( $\lambda = 8.56$  and  $12.4 \mu\text{m}$ ).

### References

- [1] F. J. G. de Abajo, "Graphene Plasmonics: Challenges and opportunities," ACS. Photonics, Vol. 1, pp. 135-152, 2014.
- [2] M. Feritag, T. Low, W. Zhu, et al., "Photocurrent in graphene harnessed by tunable intrinsic plasmons," Nat. Commun, Vol. 3, pp. 1-8, 2013.
- [3] E. H. Hwang, R. Sensarma, and S. D. Sarma, "Plasmon-Phonon coupling in graphene," Phys. Rev. B, Vol. 82, pp. 195406 (1-5), 2010.
- [4] H. Suzuura, and T. Ando, "Phonons and electron-phonon scattering in carbon nanotubes," Phys. Rev. B, Vol. 65, pp. 235412 (1-15), 2002.
- [5] F. Giustino, "Electron-phonon interactions from first principles," Rev. Mod. Phys, Vol. 89, pp. 015003 (1-63), 2017.
- [6] T. Low, V. Perebeinos, R. Kim, and et al., "Cooling of photoexcited carriers in graphene by internal and substrate phonons," Phys. Rev. B, Vol. 86, pp. 045413(1-9), 2012.
- [7] G. D. Mahan, *Many-Particle Physics*, Kluwer Academic/Plenum Publishers, pp. 323–345, 2000.
- [8] H. Yan, T. Low, W. Zhu, et al., "Damping pathways of mid-infrared plasmons in graphene nanostructures," Nat. Photonics, Vol. 6, pp. 1-6, 2013.
- [9] J. M. Jin, *Theory and Computation of Electromagnetic Fields*, Wiley, pp. 544-550, 2015.