The 26th Iranian Conference on
Optics and Photonics (ICOP 2020),
and the 12th Iranian Conference on
Photonics Engineering and
Technology (ICPET 2020).
Kharazmi University,
Tehran, Iran,
Feb. 4-5, 2020

اثرات فونون سطحی زیرلایه بر جذب پلاسمونی گرافن

شراره جلالوندی[۱]، محمدکاظم مروج‌فرشی[۱] و سارا درباری[۱]

[۱] دانشکده مهندسی برق و کامپیوتر، دانشگاه تربیت مدرس، تهران، ایران

چکیده– در مقاله‌ی پیش‌رو روش جدیدی ارائه داده‌ایم که با استفاده از آن می‌توان تأثیر زیرلایه بر جذب پلاسمونی در گرافن را با ترکیب دو روش تقریب فاز تصادفی و معادلات انتگرالی مشاهده کرد. زیرلایه‌ی قطبی 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 زیرلایه‌ی قطبی تغییر چشم‌گیری در پاشندگی ساختار ایجاد می‌کند و در نتیجه تاثیر بر روی جذب پلاسمونی نیز چشم‌گیر خواهد بود. در اینجا، ابتدا با استفاده از تقریب فاز تصادفی تابع دی‌الکتریک گرافن را بدست می‌آوریم. آشکار 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 محاسبه 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 زیرلایه‌ها 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[1], Mohammad Kazem Moravvej Farshi[2], Sara Darbari[3]

[1,2,3]Nano-Plasmo Photonics Research Group, Tarbiat Modares University, Tehran.

[1]sharareh.jalalvandi@modares.ac.ir, [2]moravvej@modares.ac.ir, [3]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 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 SiO_2 surface phonons strongly interact with the graphene surface plasmons (SPs) at the wavelengths λ =8.56 and 12.4 µm, 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_2 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_2 substrate has two surface phonons at the mid-infrared wavelengths of 8.56 and 12.4 μm, 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_2 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_{tot}, which is the sum of the external potential, V_{ext}, and the screening potential, V_{scr}. Once V_{tot} is found, the dielectric function can be obtained from

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

where ε_{RPA} is the RPA expansion of the dielectric function. To find V_{tot}, Feynman diagrams are useful. In many-particle systems with only electrons are involved, Feynman diagram looks like to Fig. 1, in which $V_{\text{C}}(q)=e^2/2q\varepsilon_0$ and $\prod_0$ 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

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

For graphene we have

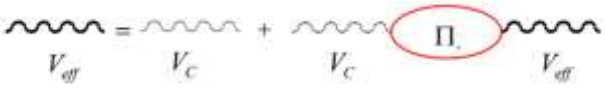

Fig. 1: Feynman diagram for a many-particle system containing only electrons.

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

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

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

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

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

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

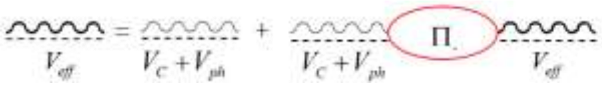

Fig. 2: Feynman diagram for a many-particle system containing electrons and phonons.

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_2 by equating them to zero, as shown in Fig. 3 when the Fermi level is 0.4 eV. As we mentioned, SiO_2 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

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

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

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

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,

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

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,

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

where σ, ε, and ε_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

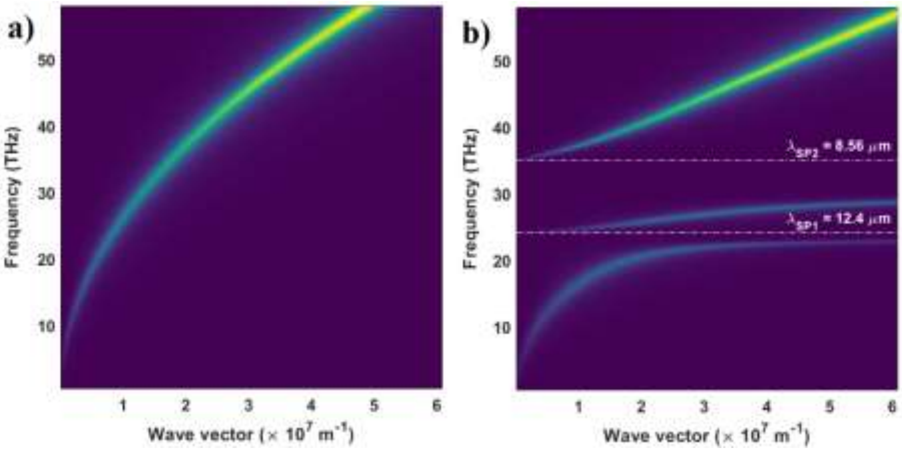

Fig 3. Plasmon dispersion for an array of graphene nanoribbons on a (a) DLC substrate with no optical phonons; and (b) SiO_2 substrate with two surface phonons.

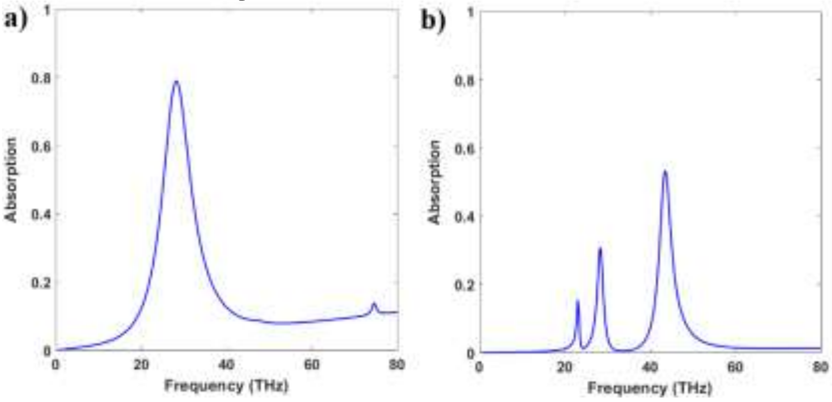

Fig 4. Plasmonic absorption for an array of graphene nanoribbons on a (a) DLC substrate with no optical phonons; and (b) SiO_2 substrate with two surface phonons.

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_2 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_2 substrate modify the graphene plasmonic absorption remarkably about the frequencies of the surface optical phonons in SiO_2 (λ = 8.56 and 12.4 μm).

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, t 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.