Tunable mid IR absorption in single-layer, nanomeshed graphene

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Abstract. Graphene, as being transparent material attempts for mid-infrared absorption. In this work, we theoretically show that excitation of localized Mid-IR plasmon resonance (LSPR) is possible in graphene single layer patterned with nano-holes. By designing graphene patterned with nanoscale holes of specific dimensions, LSPR is excited at particular wavelength, leading to noticeable absorption. We use finite difference time domain to investigate the excitation of LSPR in nano-meshed graphene at the mid IR wave length range with absorption value reaching 35 %. We also proved the excited plasmon localization at the holes’ edges through mapping the electromagnetic field distribution.

1. Introduction

Metal plasmonics have been widely investigated for mid IR absorption[1]. However, metal plasmonics encounter undeniable drawbacks including lack of tunability and high losses [2-3]. Graphene was recently demonstrated as a new emerging plasmonic material that exhibit surface plasmons in the mid IR wavelength range [4]. Graphene as being a transparent material is hardly being used for mid-infrared absorption application[5]. Only through Nano patterning of graphene into nano ribbons or nano holes- which are commonly referred as nano meshed graphene (NMG), absorption in graphene can be addressed [6-8]. Most of the previous studies have investigated NMG accompanied with back thick metallic reflectors to avoid any transmission through graphene layer[9]. Furthermore, studies have investigated nano patterned graphene in form of nano holes or nano ribbons accompanied with high induced voltage[10-12]. In this work, we show that it is possible to excite localized surface plasmon resonance (LSPR) in NMG without any external applied voltage or using metallic layers. We used Finite-difference time-domain method to investigate the excitation of LSPR in NMG at the mid-IR wave length range with high absorption values. Furthermore, we report tuning the absorption peak of the excited LSPR upon changing holes’ dimensions diameter (d) and hole period (a). We demonstrate new avenues to develop mid-IR absorption in single layer of NMG [13].

2. Design and modeling

Finite difference time domain (Lumerical) was used to study the electromagnetic field (EM) distributions of all the investigated NMG structures. The monolayer of graphene sheet was modeled as 2D layer with a dynamical surface conductivity described by surface conductivity model using the Green’s function [14].

\[
\sigma(\omega, \mu, \Gamma, T) = \sigma_{\text{intra}}(\omega, \mu, \Gamma, T) + \sigma_{\text{inter}}(\omega, \mu, \Gamma, T)
\]

\[
\sigma_{\text{intra}}(\omega, \mu, \Gamma, T) = \frac{-i\epsilon^2}{\Pi \hbar(\omega + i2\Gamma)} \int \frac{d\xi}{\xi} \left( \frac{\partial f_d^{+}(\xi)}{\partial \xi} - \frac{\partial f_d^{-(\xi)}}{\partial \xi} \right) d\xi
\]

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\[ \sigma_{\text{inel}}(\omega, \mu, \Gamma, T) = \frac{i e^2}{\hbar} (\omega + i 2\Gamma)[0, \infty] f_d^*(-\xi) - f_d(\xi) \frac{1}{(\omega + i 2\Gamma') - \mu} d\xi \]  

(3)

\[ F_d(\xi) = \frac{1}{\exp^{\left(\xi - \mu \right) / k_B T} + 1} \]  

(4)

where, \( \omega \) is angular frequency, \( \Gamma \) is a scattering term, \( \mu_c \) is chemical potential, \( e \) is electronic charge, \( \hbar \) is reduced Plank’s constant, \( K_B \) is Boltzmann constant and \( F_d(\xi) \) is the Fermi-Dirac distribution. The intra-band transition term is computed analytically while the interband transition is solved numerically.

A 2D sheet of graphene material is defined with potential of 0.22 eV which corresponds to low doped graphene deposited on quartz substrate. NMG is defined with parameters; diameter (d) = 20 nm and period (a), as can be seen in figure (1). For the simulation parameters, a TM plane wave is incident on the NMG on quartz with normal incidence. Bloch boundary conditions were applied along the direction of periodicity of the structure (x and z) whereas perfect matched layer was applied in the propagation direction (y).

![Figure 1: Schematic of the structure of the NMG on quartz substrate simulated by FDTD.](image)

3. Results and discussion

We started by investigating the excitation of LSPR in NMG on quartz substrate. Figure 2a shows the FDTD simulation results for NMG with diameter (d) 20 nm and period (a) 60 nm, at 0.22 eV potential, which yields an absorption peak at 11.1 μm. On the other hand, graphene, at the same applied potential, yields zero absorption at the same wavelength. The absorption of quartz is extracted from previous results. Figure 2b shows that there is high field confinement at the LSPR excitation wavelength concentrated at the hole edges. Generally, absorption is calculated from the following relations: \( A = 1 - (R + T) \), where \( A \) is the absorption, \( R \) is the reflection and \( T \) is the transmission. The \( R \) and \( T \) can be extracted directly from the Lumerical software yielding absolute reflection and Transmission and thus absolute Absorption as well.

We proceeded to investigate the probability of tuning the LSPR wavelength by changing the holes dimensions: (d) and (a). Figure (3a) shows the variation of the LSPR peak upon changing “a”. It can be clearly seen that as the distance between the holes is increased, the coupling strength between the plasmons of the NMG is reduced; therefore, the LSPR peak experiences a red shift. However, when the distance between two holes is reduced the LSPR peak blue shifts.
Figure 2. a) Absolute absorption of NMG and graphene without patterning, both are on quartz substrate. b) Electric field distribution of NMG at wavelength 11.1 μm showing the hole of diameter 20 nm, and period of 60 nm on Quartz substrate, the x and y are the coordinates used in Figure (1) where the field distribution were examined.

Figure 3. Absolute absorption of NMG on quartz at: a) different hole periods and b) different hole diameters.

Figure (3b) shows that upon changing the (d) of the NMG, the LSPR wavelength can be tuned as well. It can be seen that as the diameter increases the LSPR peak blue shifts due to the increase in the coupling strength. Generally, upon tuning the nano holes’ parameters, the plasmonic resonance can be tuned which confirms tunable mid IR absorption in NMG layer.
4. Conclusion

In our study, we describe a methodology to design a nano meshed graphene without the need of induced potential, external chemical doping, or even thick reflective metallic layers. We report an absorption in NMG reaching 35% at normal incidence in the mid-IR wavelength range. We further report tuning the plasmonic resonance by changing the period and the diameter of the nano holes. Our results engender new paradigms to utilize mid-IR absorption for mid IR sensing application.

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