ABSTRACT

The extremely demanding fabrication precision has been a main block for real application of nanoscale metamaterial. To overcome this, a graphene-based tunable filter has been theoretically demonstrated to exhibit generally high filtering efficiency for the filter with mismatched geometry parameters. Rigorous coupled-wave analysis has been employed to investigate the transmission spectrum and electromagnetic field distributions for TM wave. The selectivity is understood as the excitations of surface plasmon polariton (SPP), magnetic polaritons (MP) and Fabry-Perot-like (FP) resonance. The dispersion relationship of SPP and inductor and capacitor of MP are utilized to quantitatively predict the resonance wavelengths. Moreover, the propagating electron wave on the conducting surface is employed to investigate the tuning effects. The fundamental understanding gained herein facilitates the rational design of novel graphene-based metamaterials.

KEYWORDS

metasurface; nanophotonic; graphene

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1. Introduction

The urgent need in waste heat harvesting has engendered extraordinary interest in thermophotovoltaic (TPV) technology.[1,2] Selective emitters and filters can reduce a significant portion of the non-convertible radiation for the TPV cell. Recent advancements in metamaterial have provided various selective emitters and filters. Wang et al. demonstrated film-coupled concave grating metamaterial.[3] Shuai et al. reported polariton-enhanced selective thermal emitter and discussed the effect of mismatching tolerance in optical response.[4] Although selective metamaterials have been intensively studied over years, inevitable high fabrication accuracy of microstructures has limited the process of their real applications.

A great deal of work has been dedicated to graphene, a two-dimensional honeycomb like material, due to its unique properties.[5] The optical properties of graphene can be actively controlled by chemical and electrical approaches. Recently, tunable graphene-based metamaterials such as selective thermal emitter,[6] optical modulator,[7] and two-dimensional pillar arrays[8] have been investigated. In this paper, we indicate that by employing graphene, a TPV system can maintain relatively high filtering efficiency even with great fabrication mismatching in selective filter.

The paper is arranged as follows: first, the rigorous coupled-wave analysis (RCWA) and optical models used in the paper have been introduced. Second, we show the heavy geometric dependence of nanostructure and the tunability of graphene-based filter. The mechanism of selective transmission, concluded as the excitation of surface plasmon polariton (SPP), magnetic polaritons (MP), and Fabry-Perot-like resonance (FP), is also discussed in this part. Finally, the geometric effects are investigated with dispersion relation of SPP and LC model for MP are used to show the accuracy of numerical method. The mechanism for the tuning effects has also been discussed in this part.

2. Numerical methods

The structure is illustrated in Figure 1(a), a single sheet of graphene is laid atop the Ag gratings with SiO₂ layer. Considering EM wave can propagate hundreds of wavelengths with little attenuation, in this paper, the SiO₂ substrate is considered as transparent in the discussed spectral region.[7] The metallic grating with graphene covered, SiO₂ layer, and the conducting transparent substrate forms a capacitor, chemical potential of graphene

![Figure 1.](image)

Figure 1. (a) Schematic of the graphene-based tunable filter. Filtering efficiency of filter without graphene as a function of (b) groove width b, with h = 0.4 μm, P = 0.5 μm, (c) grating height h, with b = 0.05 μm, P = 0.5 μm, and (d) grating period P, with b = 0.05 μm, h = 0.4 μm.
can be dynamically tuned by applying the voltage between graphene and substrate. The Ag grating and the conducting substrate play the role of electrodes, and the static electric field inside the cavity directly controls the electro-optical response inside the graphene. The metallic grating and the graphene on it consist of a tunable metasurface whose radiative property can be actively controlled. The thickness of the grating layer is $h$; the period and groove width of the one-dimensional gratings are $P$ and $b$, respectively. $E_{b,\lambda} (\lambda, T)$, is the spectral power density of blackbody defined as [9]:

$$E_{b,\lambda} (\lambda, T) = \frac{2 \pi \hbar c^2}{\lambda^5} \left( e^{\hbar c / \lambda k_B T} - 1 \right)$$  \hspace{1cm} (1)

The waste heat emitter is assumed as black body and the temperature is set as 1000 K. The overall transmission power density of filter is defined as [10]:

$$P_{\text{total}} = \int_0^{\infty} \tau(\lambda) E_{b,\lambda} (\lambda, T) d\lambda$$  \hspace{1cm} (2)

Here $\tau(\lambda)$ is the hemispherical spectral transmittance of the filter. The radiant power within the convertible wavelength of TPV cell is defined as:

$$P_{\text{inband}} = \int_0^{\lambda_i} \tau(\lambda) E_{b,\lambda} (\lambda, T) d\lambda$$  \hspace{1cm} (3)

where $\lambda_i$ is the bandgap wavelength and the bandgap is set as 0.53 eV as InGaAsSb TPV cell. [11] For simply research, the quantum efficiency of the TPV cell is set as 100%. The far-field TPV filtering efficiency can be expressed as:

$$\eta_{\text{sys}} = \frac{P_{\text{inband}}}{P_{\text{total}}}$$  \hspace{1cm} (4)

As being demonstrated by various previous results, TE-polarized wave contributes slightly to the spectral selectivity,[1,4,6,8,12,13] and the mechanism for the spectral selectivity is quite similar for TM wave and 2D structures. In this work, only TM-polarized wave has been investigated.

The accuracy of the solution provided by RCWA solely depends on the order of the space-harmonic expansion of the field. To balance the computation time and accuracy, we choose the order of ±300 to obtain reasonable convergence in our 2D RCWA calculation. The diffraction order $N$ is chosen as 300 to predict the optical response accurately. Ag is modeled with a Drude model with dielectric function: $\varepsilon_{\text{Ag}} = 1 - \omega_p^2 / (\omega^2 + i \gamma \omega)$ with plasma frequency $\omega_p = 1.37 \times 10^{16}$ rad s$^{-1}$ and scattering rate $\gamma = 2.73 \times 10^{11}$ rad s$^{-1}$. The monolayer graphene is modeled as a thin film whose dielectric function is given by: $\varepsilon_{\text{G}} = 1 + i \sigma (\omega \Delta \varepsilon_{\text{G}})$, where the effective thickness $\Delta = 0.3$ nm, $\omega$ is the angular frequency, and $\varepsilon_{\text{G}}$ is the vacuum permittivity. The optical conductivity of graphene $\sigma$ includes intraband and interband contributions (Drude-like) $\sigma = \sigma_{\text{inter}} (\omega, \mu, T) + \sigma_{\text{Drude}} (\omega, \mu, T)$, which depend on the temperature $T$, electron relaxation time $\tau$, and chemical potential $\mu$, and is given as [12]:

$$\sigma_{\text{inter}} = \frac{e^2}{4\hbar} \left[ G(\hbar \omega) + \frac{4 \hbar \omega}{\pi} \times \int_{\eta=0}^{\infty} \frac{G(\eta) - G(\hbar \omega/2)}{\hbar \omega^2 - 4 \eta^2} d\eta \right]$$  \hspace{1cm} (5)

$$\sigma_{\text{Drude}} = \frac{i}{\omega + i/\pi \hbar} \frac{e^2}{2k_B T} \cdot \ln \left[ 2 \cosh \left( \frac{\mu}{2k_B T} \right) \right]$$  \hspace{1cm} (6)

where $G(\eta) = \sin(\eta/k_B T)/[\cosh(\eta/k_B T) + \cosh(\mu/k_B T)]$. The conductivity is calculated by setting $\tau = 10^{-13}$ s and the temperature of filter is set as 300 K. The applied voltage is defined by $\mu = 2hV_\eta (\eta | V' + V_0 |)^{0.5}$, where Fermi velocity $V_\eta$ is $9.96 \times 10^6$ m s$^{-1}$, voltage offset caused by natural doping $V_0$ is $-0.8$ V, and $\eta = 9 \times 10^{16}$ m$^{-2}$ V$^{-1}$ is estimated from capacitor.[7]

3. Results and discussions

3.1. The geometric dependences of filtering efficiency and the tunable zone of filter

The filtering efficiency of filter without graphene as functions of geometric parameters is shown in Figure 1(b)–(d). All three plots show single filtering efficiency peak with specific matching geometric parameters. In Figure 1(b) with $b = 0.08$ μm $\eta_{\text{sys}} = 0.58$, in Figure 1(c) with $h = 0.65$ μm $\eta_{\text{sys}} = 0.32$, and in Figure 1(d) with $p = 1.7$ μm $\eta_{\text{sys}} = 0.31$, but the filtering efficiency might approach to 0 if geometric parameters are badly matched. For a system consisted of numerous blocks of TPV, varying filtering efficiency can generate potential differences between blocks not considered in the blueprint. Such potential differences will weaken the system’s stability and may even to lead to overall failure of system. Such results indicate that the demanding matched geometric parameters are essential for metamaterials to exhibit desired properties, which limits the fabrication and application of them. To build a TPV system, filtering efficiency of every block should be restricted to a certain range.

To overcome such problem, the concept of tunable zone has been introduced in this paper. By changing the voltage, the filtering efficiency of tunable filter can be localized in a certain range. Tunable zone is up to the fabrication tolerance and objective efficiency range. To evaluate geometric
$$q = 1.27 \quad (b) \quad \eta_{sys} = 0.3 \pm 0.1, \quad q = 0.97 \quad (c) \quad \eta_{sys} = 0.38 \pm 0.08, \quad q = 0.86.$$
3.3. Analytical models and the mechanism for the tunable selectivity

In periodic grating, when the in-plane wave vector satisfies the dispersion relation as [9]:

$$|k_{spp}| = \frac{\omega}{c_0} \sqrt{\frac{\varepsilon_1 + \varepsilon_2}{\varepsilon_1 \varepsilon_2}} = |k| = k_{inc} + \frac{2\pi m}{\lambda}$$  (7)

SPPs can be excited in the interface of two dissimilar materials with permittivity $\varepsilon_1$ and $\varepsilon_2$. Where $m$ is the diffraction order in x direction and in the normal incident $k_{inc} = 0$. The LC model applied in the paper is depicted in Figure 5(a). By zeroing the total impedance, the resonance wavelength of MP can be obtained as $\lambda_{MP} = 2\pi [(2L_{Ag} + 2L_m + L_{SiO_2})/C]^{0.5}$. The air inside the slit acts as a capacitor with a capacitance of $C = c_1\varepsilon_1 h/b$, where $c_1 = 0.3$ is the coefficient responsible for the non-uniform charge distribution.[8] The mutual inductance is given as $L_m = \mu h b/2$. The Ag walls around the ridges serve as conductors, with inductances expressed as:

$$L_{Ag} = -\frac{h}{\varepsilon_0 \omega^2 \delta} \frac{\varepsilon_A' \varepsilon_A''}{\varepsilon_A' + \varepsilon_A''}$$  (8)

As shown in Figure 4(c), for FP, $H$ field is enhanced in the surface between cavity and substrate. The enhanced $H$ field is associated with the equivalent dipole $P_b$. The incident beam exerts driving force on electrons on the surface on the top of conductive slit wall. The propagation of charge wave is impeded at the corners of the slit and electrons tend to accumulate there. Then the electrons highly accumulated around the corner produce mutual opposite current on the surface of ridges. When the charge waves propagating along the wall approach to the end of the slit, they are impeded once again around the corners. On the bottom corners of the groove, the electrons are accumulated forming dipole $P_b$, which forms the transmitted beam. [13] Moreover, in the bottom of the slit, the lack of vertical driving forces makes the surface wave stop on the end of the walls. The charge wave is alternatively bounced back between the top and the bottom of the ridges, which form the so-called FP. The energy transport discussed above is involved with the movement of electrons on the conducting surface, the groove plays the role of energy flow path thus the importance of graphene’s conductance on electron-electromagnetic wave energy transfer process could not be exaggerated.[6,12]
The geometric parameters but the graphene’s chemical potential affects it slightly, which is previously reported in [12]. In oscillating MP, the E field has been enhanced inside the slit, wherein the graphene has not been involved in the resonance. This phenomenon has also been verified by the LC model.

As FP is induced by the electron wave alternatively bouncing in the slit wall and making grooves a energy flow path, it is observed that flowing path-associated factors, groove width, height, and optical conductance, influence the resonance condition of FP, but not the grating period. In Figure 5(e), spectral transmission of FP and the background around it can be changed by varying the applied voltage. The EM wave inside the slit, associated with the charge wave along the wall, is induced by the accumulated electrons around the corners. The conducting graphene on the top of the grating can weaken such accumulation and let the charges neutralized. The optical conductivity of graphene generally increases with applied voltage in the infrared region as discussed in the paper [8]. The increased optical conductivity of graphene would make the charges further neutralized. Also, the conducting graphene can change the propagation of charge wave on the top of the grating, so that the resonance condition of FP can further be controlled.

\[ \delta = \frac{\lambda}{4\pi\kappa} \]

where \( \delta \) is the penetration depth, \( \kappa \) is the extinction coefficient of Ag. The LC model and dispersion relation show good agreement with RCWA calculation in Figure 5, indicating the accuracy of numerical method.

In the spectral range discussed in the present study, three types of resonances, SPP, MP, and FP have been excited. The next question is which of them has made dominating contribution to the tuning effect. The filtering efficiency studied in this paper is defined as the ratio of convertible radiation and the total. Thus, the tuning FP can maintain the filtering efficiency by deducting the transmission of inconvertible. In this case, SPP and MP have contributed slightly to the tuning effect and the FP is the dominant one. In Figure 5, neither the groove’s height and width nor applied voltage has enormous affections on the resonance wavelength of SPP. That is because SPP is excited when the incident waves are oscillating with the grating scattering in plane vectors, so we can see a positive correlation between the resonance wavelength and grating period (Figure 5(d)). Also, surface waves propagate along the interface between dielectric layer and metallic grating, thus graphene laid atop the grating affects the resonance condition of SPP slightly. For MP, the resonance wavelength is heavily dependent on the geometric parameters but the graphene’s chemical potential affects it slightly, which is previously reported in [12]. In oscillating MP, the E field has been enhanced inside the slit, wherein the graphene has not been involved in the resonance. This phenomenon has also been verified by the LC model.

As FP is induced by the electron wave alternatively bouncing in the slit wall and making grooves a energy flow path, it is observed that flowing path-associated factors, groove width, height, and optical conductance, influence the resonance condition of FP, but not the grating period. In Figure 5(e), spectral transmission of FP and the background around it can be changed by varying the applied voltage. The EM wave inside the slit, associated with the charge wave along the wall, is induced by the accumulated electrons around the corners. The conducting graphene on the top of the grating can weaken such accumulation and let the charges neutralized. The optical conductivity of graphene generally increases with applied voltage in the infrared region as discussed in the paper [8]. The increased optical conductivity of graphene would make the charges further neutralized. Also, the conducting graphene can change the propagation of charge wave on the top of the grating, so that the resonance condition of FP can further be controlled.
4. Conclusion

In summary, we have numerically demonstrated graphene-based tunable filter in the infrared region. Such device could sustain generally high filtering efficiency even with great geometric mismatching for TM wave. The EM field distributions have revealed the SPP, MP, and FP as the underlying mechanism for the selective transmission. The tuning effects are understood from the behavior of electron wave propagating on metallic surface and the effects caused by conducting graphene. LC model and SPP dispersion relationship are utilized to confirm the accuracy of numerical method. This study will facilitate the utilization of nanostructure in real manufacture and the basic understanding of graphene-associated tunability.

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Disclosure statement

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