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Ultra-wide Spectral Bandwidth and Enhanced Absorption in a Metallic Compound Grating Covered by Graphene Monolayer

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Abstract— Graphene, a two-dimensional monatomic layer of carbon material, has demonstrated as a good candidate for applications of ultrafast photodetectors, transistors, transparent electrodes, and biosensing. Recently, many studies have shown that using metallic deep gratings could enhance the absorbance of graphene of 2.3% up to 80% in the near infrared region for applications in photon detection. **This paper presents utilizing a nanograting structure, namely, a compound metallic grating could greatly enhance the absorbance of graphene up to 98% and widen its spectral bandwidth to 0.6 μm , which are greater than those of previous work.** The study also showed that the absorbance spectrum is insensitive to angles of incidence. Furthermore, the proposed graphene-covered compound grating might bring a lot of benefits for graphene designs-based optical and optoelectronic devices.

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I. INTRODUCTION

GRAPHENE is a two-dimensional (2D) material with carbon atoms arranged in a honeycomb lattice, and it offers many potential applications for optoelectronic devices due to its unique electrical, mechanical, and optical characteristics [1-8]. To be detailed, the electrons in graphene are known as massless quasi-particles exhibiting a linear energy dispersion. More importantly, a very high carrier mobility (larger than $200,000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$) makes graphene as an excellent material used for ultrafast photodetectors and transistors in the visible and near infrared (NIR) regions [2, 7, 8]. Unlike transistors, the photon detectors are designed with a requirement of strong light absorbance which generates more electro-hole pairs, and it thus produces a greater photocurrent [7, 9-11].

As demonstrated, optical properties of graphene in the mid- and far-IR are similar to those of Drude-type materials and make strong resonance absorption when graphene interacts with light due to its plasmonic resonance [12-17]. On the other hand, in the visible and NIR ranges, there is no plasmonic response, and the absorption of a single-layered graphene is about 2.3% due to its very thin thickness [18]. Accordingly, absorption enhancement is necessary for the application of photon detection based on graphene designs. Many methods of the absorption enhancement have been proposed by using microcavities and nanostructures [7, 19-31]. A microcavity enhances absorption by allowing light to pass through the graphene layer multiple times [7]. **Meanwhile, a deep grating structure covered by a graphene sheet could also enhance absorbance due to a strong localized electric field causing the magnetic resonances [9, 23, 24, 32, 33]. Although this grating exhibits absorbance of 81% and a spectral bandwidth of 0.3 μm , it is very sensitive to angles of incidence [23, 24]. Accordingly, novel structures featuring a higher absorbance, a wider bandwidth and independence on angles of incident light are still in need. One of the simple gratings, namely a single-layered compound grating (CG) has not yet been studied and utilized to increase the absorption of graphene and widen its spectral bandwidth.**

In the present study, we propose CGs used to enhance graphene absorption, and its enhancement is caused by strong localized electromagnetic fields inside grating trenches and surface plasmons. A CG has a several multiple grating periods [34], and it is also named as a double-period grating, a

dual-pitch grating, a dual-period grating or a complex grating [35-38]. On the contrary, a simple grating (SG) has a single grating period [17]. Figure 1 (a) shows the schematic of a silver (Ag) SG structure while Fig. 1(b) similarly illustrates an Ag grating but covered by a graphene sheet on the top. As demonstrated in previous studies, graphene covered on SG structures works as a pure conductor or resistor in the NIR region which could absorb a large of incidence energy at the trench opening of deep gratings [23]. In addition to that, it was seen that resonance wavelengths in the SG structures and the structures covered by a graphene sheet remain unchanged. Accordingly, in order to enhance the absorption of graphene, this manuscript presents an optimal analysis of the absorptance of different SG structures. Their geometries are then tailored to have CG structures that could significantly elevate the absorption and their physical phenomena are investigated as well.

II. MODELING DEVELOPMENT AND NUMERICAL METHOD

A. Geometric Grating Structure

As shown in Fig. 1(a), the geometry of the SG structure is defined by the period (Λ), the lamella width $w\Lambda$ (w is the filling ratio, $0 < w < 1$), and the grating thickness (d). Similarly, Fig. 1(b) shows the same SG but covered by a graphene layer (at $z = 0$) with a thickness of h . The incident transverse magnetic (TM) \mathbf{H} travels through free space with an orientation defined by the polar angle θ between the wavevector \mathbf{k} and the surface normal z . For the one-dimensional gratings shown in Fig. 1, the electromagnetic field is independent to y -axis because the wavevectors of all diffracted waves lie in the x - z plane, and thus, there are no excitations in the y direction. **In this study, the TM wave is used for calculations because as theoretically and experimentally demonstrated designer surface plasmons (SPPs) or Fabry-Perot modes could be excited when the TM polarization is applied in the y direction [17, 23, 24, 34, 39-42].** The Ag base below the grating is assumed to be thick enough as an opaque. Accordingly, the transmittance is equal to 0, and the absorptance (α) can be computed from the reflectivity (R) via $\alpha = 1 - R$, where the reflectivity was calculated by the rigorous coupled-wave analysis (RCWA) based on a home-made program [43].

B. Numerical Method

In the simulation, the optical property of Ag is calculated based on a Lorentz-Drude model [43] [44] expressed as:

$$\varepsilon(\omega) = \varepsilon_{r,\infty} + \sum_{k=0}^K \frac{f_k \omega_p^2}{\omega_k^2 - \omega^2 + j\omega\Gamma_k} \quad (1)$$

where $\varepsilon_{r,\infty}$ is the dielectric constant at infinite frequencies, ω_k , f_k and Γ_k are the resonance frequency, strength and damping frequency of the k th oscillator, and ω_p is the plasma frequency. These values of Ag are taken from [44]. Meanwhile, the dielectric function of graphene is described as $\varepsilon(\omega) = 1 + i\sigma_s / (\varepsilon_0 \omega h)$ [6], where σ_s , ε_0 , and ω are the sheet

conductivity, the vacuum permittivity, and the angular frequency, respectively. The sheet conductance σ_s ($\sigma_s = \sigma_D + \sigma_I$) including the contribution of a Drude (intraband) term σ_D and an interband term σ_I is described as:

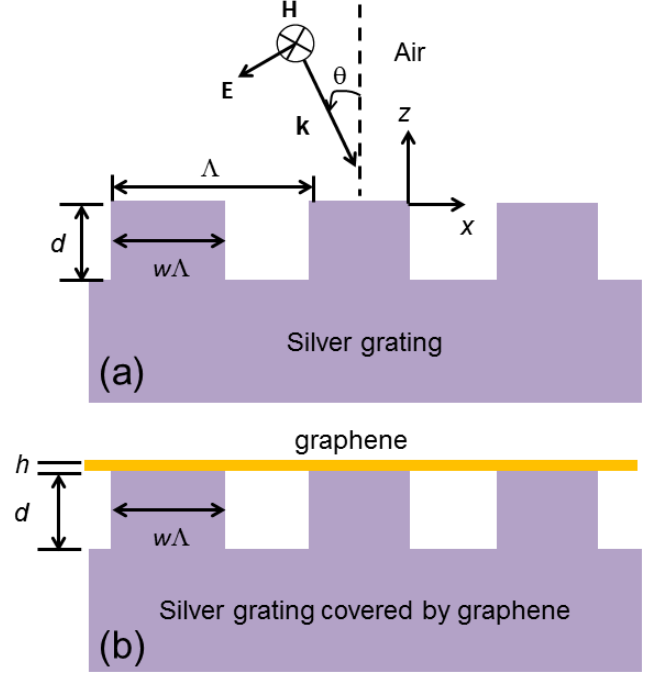


Fig.1. Schematic illustration of (a) grating structure and (b) graphene-covered Ag grating. Their geometries are defined by grating period Λ , grating thickness d , lamella width $w\Lambda$ (w is filling ratio), and graphene thickness h . The transverse magnetic wave \mathbf{H} (parallel to the grating grooves or y -axis) is incident on the grating with a wavevector \mathbf{k} and an angle θ

$$\sigma_D = \frac{i}{\omega + i/\tau} \frac{2e^2 k_B T}{\pi \hbar^2} \ln \left[2 \cosh \left(\frac{\mu}{2k_B T} \right) \right], \quad (2)$$

and

$$\sigma_I = \frac{e^2}{4\hbar} \left[G \left(\frac{\hbar\omega}{2} \right) + i \frac{4\hbar\omega}{\pi} \int_0^\infty \frac{G(\xi) - G(\hbar\omega/2)}{(\hbar\omega)^2 - 4\xi^2} d\xi \right], \quad (3)$$

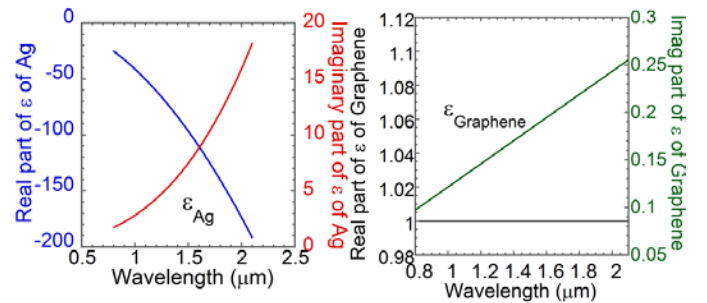


Fig.2. Real and imaginary parts of the permittivity of Ag and graphene. It is noted that the permittivity of graphene is computed based on $\mu = 0.3$ eV, $\tau = 10^{-13}$ s, $T = 300$ K, and $h = 0.3$ nm

where $G(\xi) = \sinh(\xi/k_B T) / [\cosh(\mu/k_B T) + \cosh(\xi/k_B T)]$ [14]. In the above equations, e is the electron charge, \hbar is the

reduced Planck constant, and k_B is the Boltzmann constant. Other parameters are used for the calculation such as the Fermi energy $\mu = 0.3$ eV, relaxation time ($\tau = 10^{-13}$ s), the temperature $T = 300$ K, and the thickness of graphene, $h = 0.3$ nm. It is noted that the Fermi energy, $\mu = 0.3$ eV, was used in the current work because calculations have shown that with this selected value in a range of 0.2 to 0.5 eV graphene-covered grating structures exhibit the highest absorptance. Accordingly, the property of graphene can be changed by varying μ which results in a change of plasmonic resonances [33]. Meanwhile, the optical property of Ag based on the Lorentz-Drude model and graphene is plotted in Fig. 2. It is seen that, the real part of permittivity of Ag decreases when the incident wavelength increases while that of graphene is constant. On the contrary, the imaginary part of permittivity of Ag rises when the incident wavelength goes up, and the imaginary part of graphene has a similar trend.

III. NUMERICAL RESULTS AND DISCUSSION

A. Absorptance Spectrum at Normal Incidence

Figure 3 shows the absorptance contours for TM waves at normal incidence of two types of gratings: (a) and (b) the short period grating with and without a graphene overlay, and (c) and (d) the long period grating with and without a graphene layer as a function of wavelength and filling ratio w ($0 < w < 1$), respectively. The short period, $\Lambda = 140$ nm, is to be divided in 7 sections while the long period, $\Lambda = 540$ nm, is divided into 27 sections. For instance, each lamella width (one section) corresponds to 20 nm ($w\Lambda = 20$ nm, and so $w = 1/7 = 0.14$ for the short period grating and $w = 1/27 = 0.04$ for the long period grating), and the grating thickness d is 200 nm while that of graphene h is 0.3 nm. The above values of the lamella width and the grating thickness are selectively feasible for fabrication since their aspect ratio 1:10 is satisfied with current manufacturing techniques. For example, to manufacture gratings one could use a cryogenic etching method to etch deep grating trenches to have the desired geometric gratings and then transfer the graphene onto the gratings. Previous fabrication processes were implemented with a deep width to wall thickness ratio (aspect ratio) up to 40 and a possible trench width of 20 nm [45-47]. Note that graphene is fabricated using chemical vapor deposition on a copper foil. In order to validate our RCWA MATLAB codes, we repeated calculations of radiative properties for the graphene-covered deep grating in Ref. [24], and results (not shown here) have revealed that our obtained absorptance and that of this structure are well-agreed.

As can be seen from Fig. 3 (a) and (c), the absorptance α is obtained to be high at the larger filling ratio at $w = 6/7 = 0.86$ for the short period grating ($\alpha = 0.3$ at the peak $\lambda = 1.67$ μm) and $w = 25/27 = 0.93$ for the long period grating ($\alpha = 0.6$ at the peak $\lambda = 1.47$ μm), and there is no absorptance at small filling ratios. It can be revealed that when the trench (containing air) is opened wider (the lamella width is thus smaller), the absorptance decreases significantly. On the other hand, the trench gets smaller the higher absorptance is obtained due to the coupling of surface plasmons and localized magnetic fields

trapped in grating trenches. Results (not presented here for simplicity) have shown that the SPP occurs at the interface of Ag and air surroundings, and standing waves oscillate in the grating trenches of the short period grating structure [as shown in Fig. 3(a)] with $w = 6/7$ (narrow slits). In contrast, there were no resonance modes to be observed in the short period one with large slits (e.g., $w = 0.14$). The results were in agreement shown in previous work [23, 24, 34, 48]. The structural grating was also optimized with different thicknesses to get an optimal small trench (with $d = 200$ nm) and to ensure for the ease of fabrication as well. Similarly, the absorptance of the graphene-covered Ag short period and long period gratings in Figs. 3(b) and (d) are much enhanced compared with that shown in Figs. 3(a) and (c). In general, Fig. 3 provides a good guideline for designing gratings-based graphene with high optical absorptance.

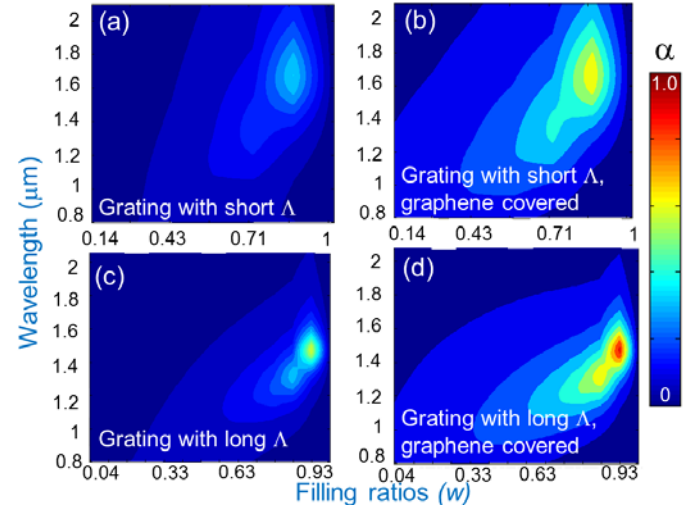


Fig. 3. Absorptance (α) contours at normal incidence for (a) short period Ag grating with $\Lambda = 140$ nm, (b) graphene-covered Ag grating with short $\Lambda = 140$ nm, (c) long period Ag grating with $\Lambda = 540$ nm, and (d) graphene-covered Ag grating with long $\Lambda = 540$ nm in terms of filling ratio ($0 < w < 1$) and wavelength λ .

Figure 4 (a) shows the normal-incidence absorptance of the short and long period gratings with and without a covered graphene sheet with the periods of 140 nm and 540 nm, respectively. It is noted that the short period grating and long period grating with filling ratios of 0.86 ($w = 6/7$) and 0.93 ($w = 25/27$), respectively, the grating thickness d of 200 nm, and the graphene thickness of 0.3 nm were selected. This is because their absorptance displays high values of 0.3 at $\lambda_{\text{peak}} = 1.67$ μm and 0.6 at $\lambda_{\text{peak}} = 1.47$ μm , respectively. However, when covering a graphene layer on top of the grating structures, their absorptance increases up to 0.7 for the short period grating and 0.9 for the long period grating without changing the peak wavelengths. Figures 4(b) and (c) illustrate the absorptance contours of the short and long period graphene-covered Ag gratings in terms of the wavelength and angles of incidence. It is seen that the absorptance of the short period graphene-covered Ag grating remains high absorptance up to 40° and then drops slowly to 70° , but the absorptance spectrum with a bandwidth of 0.2 μm still covers a wide range of the incidence wavelength. Meanwhile, the absorptance with its bandwidth of 0.3 μm of the long period graphene-covered Ag

grating is insensitive to angles of incidence up to 50° and decreases slowly to 80° . In general, the absorptance of the graphene-covered gratings was much enhanced, and their spectra covered a wide range of the incident angles. However, both their absorptance and spectral bandwidths were not obtained to be higher and wider enough.

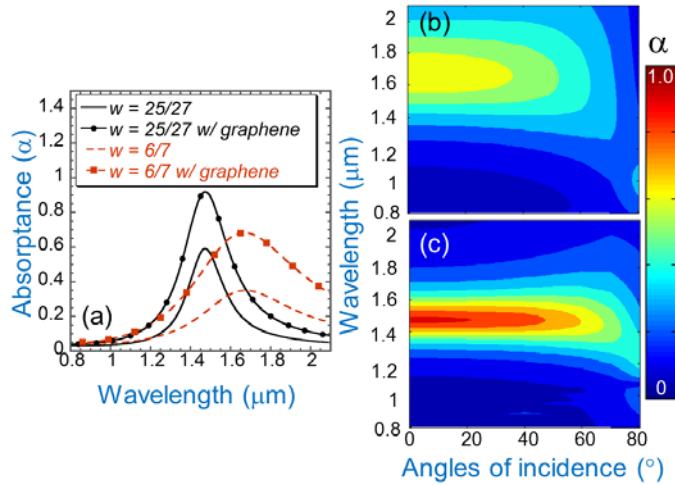


Fig. 4 (a) Normal-incidence absorptance of short period grating ($w = 6/7$, $\Lambda = 140$ nm) with and w/o graphene and long grating period ($w = 25/27$, $\Lambda = 540$ nm) with and w/o graphene, (b) and (c) Absorptance contours of graphene-covered short period and long period gratings, respectively, as function of wavelength and angle of incidence

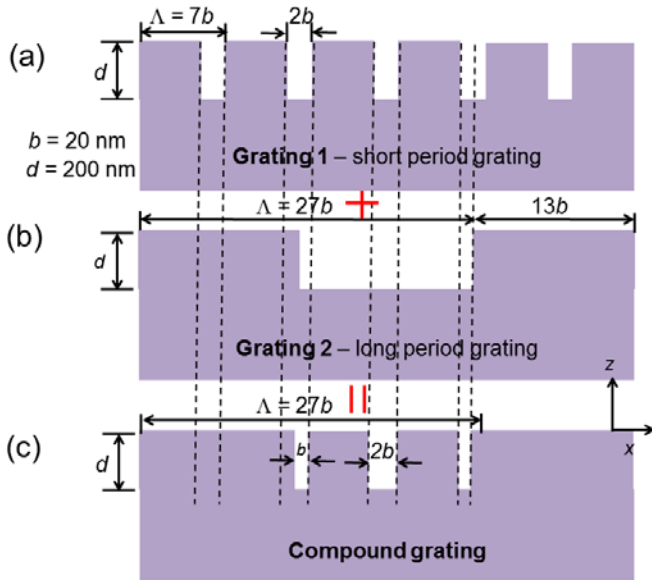


Fig. 5. Schematic illustration of (a) optimal short period grating structure and (b) optimal long period grating structure, and (c) compound Ag grating constructed based on two simple gratings. Their geometries and coordinates are similarly defined as in Fig. 1 such as grating period Λ , grating thickness d , and trench width b . Transverse magnetic wave \mathbf{H} (parallel to the grating grooves or y-axis) is incident on grating with wavevector \mathbf{k} and angle θ

Figure 5 shows the schematic illustration of (a) the short period, (b) long period, and (c) compound grating structures. The compound grating in Fig. 5(c) is constructed based on the SGs (a) and (b), and their geometries and coordinates are same as shown in Fig. 1. As demonstrated in Figs. 3 and 4, the maximum absorptance could be obtained in the short period

and long period gratings with a condition of the small trench (the filling ratio is large), e.g. $w = 6/7$ and $25/27$. Accordingly, a compound grating structure was proposed by combining this feature of two grating structures with different grating periods as shown in Fig. 5(c). Note that the short and long periods were based on the above calculation due to their high optical performance. It is also ensured that the characteristic of the trench width in the compound grating is kept to be small (the trench width was selected to be $b = 20$ nm). Therefore, the compound grating used to be analyzed features a long period of 540 nm comprising three Ag lamellae and three trenches occupied by air with different sizes.

TABLE I. COMPARISON OF OPTICAL PERFORMANCE OF PREVIOUS STRUCTURES COVERED BY GRAPHENE WITH THE CURRENT WORK

Ref.	Absorptance (%)	Spectral bandwidths (μm)	Structures
[23, 24]	81	~ 0.30	A binary grating
[26]	80	~ 0.02	Multiple layered structure
[27]	65	~ 0.12	2D nanopillars
[28]	90	~ 0.32	A metal layer with an array of groove rings covered by 8 graphene sheets
[29]	~ 50	~ 0.35	A multiple layered metal dielectric metal structure
[30]	90	~ 0.5	A metal/dielectric/metal structure
[31]	99	~ 0.02	A 2D multiple layered structure with a cross-shaped groove air resonator
This work	98	~ 0.6	A compound Ag grating

Figure 6(a) displays the normal-incidence absorptance for TM waves of the short period ($w = 5/7$), long period ($w = 13/27$), and compound gratings with and without a covered graphene layer. The compound grating was built based on the short and long period gratings. It is noted that building the compound grating having small trenches but comprising multiple lamellae and trenches requires a SG structure with a wide trench width to be superimposed by another with smaller trenches as shown in Fig. 5. Accordingly, the optimal filling ratios were selected based on Fig. 3 for calculations such as $w = 5/7$ and $13/27$. From Fig. 6(a), it is seen that the absorptance of the long period grating with a wide trench ($b = 280$ nm) is found to be 0.05 and increases to 0.22 when covered by a graphene sheet. Meanwhile, the short period grating with a trench $b = 40$ nm absorbs energy about 0.2, and this absorptance goes up to 0.4 when it is added with a graphene layer. On the contrary, the compound grating exhibits very high absorptance of 0.9 at the peak $\lambda = 1.67 \mu\text{m}$ and spectral bandwidth about $0.3 \mu\text{m}$. Interestingly, it absorbs the maximum

energy of 0.98 at the same peak wavelength when covered by a graphene sheet. In addition, its spectral bandwidth is obtained to be approximately 0.6 μm .

In order to prove superior performance of the proposed device, Table 1 shows a comparison of the optical characteristics including absorptance, bandwidths and structural geometries of previously designed structures covered by graphene and the current work. It is seen that the proposed device features a simply geometric structure exhibiting a higher absorptance (98%) and a wider bandwidth (0.6 μm) compared with those of the previous structures. Although some of previous devices have high absorptance from 90% to 99%, they own complex geometric structures (multiple layers or 2D geometries), which need more materials and complicated fabrication processes.

Figures 6(b) and (c) show the normal-incidence absorptance contours of the compound grating with and without a covered graphene layer as a function of wavelengths and angles of incidence. It is revealed that the absorptance in both structures is independent to the incident angles in a wide range from 0° to 80° . It can be observed that the grating without the graphene overlay keeps maximum absorptance at a very large range of incident angles although it exhibits a narrower bandwidth. In other words, the absorptance spectrum of the graphene-covered compound Ag grating has the wider bandwidth covering a range of wavelengths from 1.4 μm to 1.8 μm up to 40° and is then narrower after 50° . Generally, the proposed absorber provides very good optical performance, i.e. the superior absorptance, the wider spectral bandwidth, and insensitivity of the incident angles. In addition to that, it owns an easy fabrication process due to the simple structural geometry that results in cost effectiveness.

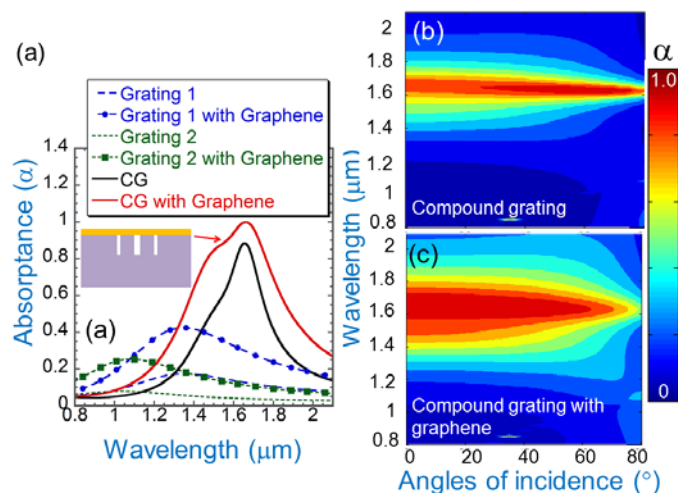


Fig. 6. (a) Normal-incidence absorptance of short period grating ($w = 5/7$), long grating period ($w = 13/27$), and compound grating constructed by superimposing short and long period grating with and w/o a covered graphene, (b) and (c) Absorptance contours of compound Ag grating and graphene-covered compound Ag grating, respectively, as function of wavelength and angles of incidence

B. Physic Origin Underlying the Grating Structures

Figure 7 shows the electric field and Poynting vector distributions in one grating period of the CG and

graphene-covered CG structures at an off-resonance wavelength of 1 μm , on-resonance wavelength of 1.67 μm , and normal incidence. Figs. 7(a) and (b) display the electric field distributions at the off-resonance wavelength corresponding to the lowest absorptance of the CG with and without a graphene layer as plotted in Fig. 6(a). As shown, the electric fields are strongly confined in the middle trench of one grating period of the CG and the graphene-covered CG structure; however, they are much enhanced at the corners of the graphene and trench opening. In other words, at the on-resonance wavelength as shown in Figs. 7(c) and (d), the electric fields trap in the two grating trenches, which results in a higher absorptance compared with those at the off-resonance wavelength. Similarly, magnetic fields (not shown here) oscillating much more in the centers of two grating trenches at the on-resonance wavelength were also observed.

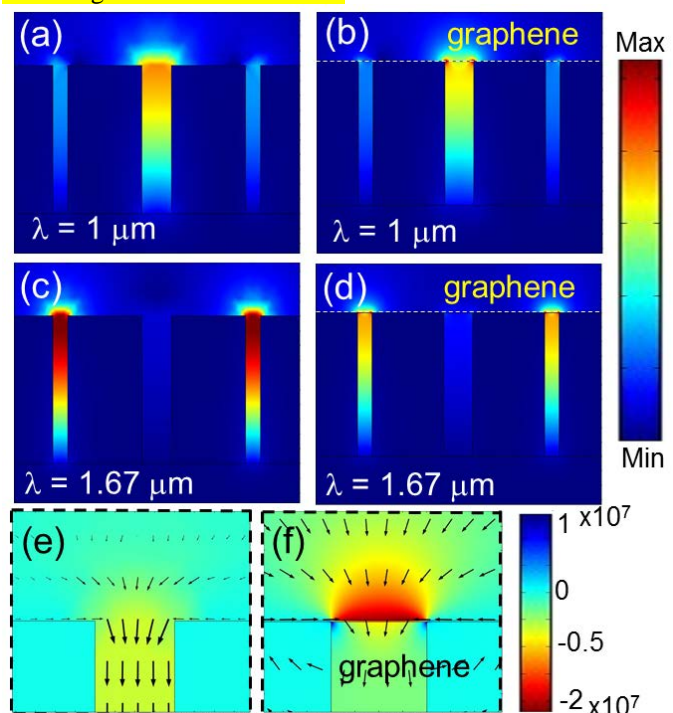


Fig. 7. Electric field distributions and Poynting vector in one grating period including three trenches of CG and graphene-covered CG structures at off-resonance wavelength ($\lambda = 1 \mu\text{m}$ and $\theta = 0^\circ$) and on-resonance wavelength ($\lambda = 1.67 \mu\text{m}$ and $\theta = 0^\circ$). (a) and (b) normalized electric field at 1 μm , (c) and (d) normalized electric field at 1.67 μm , and (e) and (f) Poynting vector patterns and arrows at 1.67 μm . It is noted that Figs. (e) and (f) show only one trench opening w/o graphene of the CG structure.

It is clearly seen from Figs. 7(a)-7(d) that high concentration of the electric fields is at the graphene and trench opening; as a result, the absorptance of graphene is elevated. This enhancement can be explained based on the power dissipation density of graphene, which is related to optical constants of graphene (high imaginary part in the permittivity) and the high electric field [24]. It is described as:

$$w(x, z) = \frac{1}{2} \varepsilon_0 \omega \varepsilon''(x, z) |\mathbf{E}(x, z)|^2 \quad (4)$$

where \mathbf{E} is the complex electric field, and ε'' is the imaginary part of the permittivity of graphene. Finally, the absorptance of graphene is calculated by dividing the power dissipated in graphene to the incident power.

Figures 7(e) and (f) show energy flowing indicated by patterns and arrows in trench opening of CG with and without graphene at normal incidence and the on-resonance wavelength, $\lambda = 1.67\mu\text{m}$. As can be seen, the energy squeezes into the trench of all the grating structures. However, the coming energy concentrates much on the interface between the graphene layer and the top edge of the trench opening. In addition, the energy flows on the surfaces of the metal layer and the graphene layer as indicated by the arrows. This confirmed that the designer surface plasmons occur at the interface of Ag (graphene) and the dielectric layer [40]. Further, energy reflects back from the grating walls and trench bottom hitting the graphene overlay; accordingly, this results in a reflection reduction. Therefore, as demonstrated the graphene layer absorbs much energy due to the localized electromagnetic fields inside the grating trench (the Fabry-Perot mode) coupling with surface plasmons [41, 49, 50]. These phenomena cause the increase of the absorptance of the whole structure and widen the spectral bandwidth as well.

IV. CONCLUSIONS

This work theoretically presented a method of enhancing graphene absorption by proposing a compound metallic grating structure. The enhancement of absorptance up to the maximum attainable of 100% was demonstrated with the observation of strongly localized electromagnetic fields in the grating trenches and SPP modes at the interface of Ag/graphene and air. Moreover, the resonance frequency occurred in the compound Ag grating with and without a graphene overlay remains unchanged. It has also shown that the spectral bandwidth of 0.6 μm is found to be wider than that of the previous studies, and the absorption spectrum is insensitive to a large range of the angles of incidence. Additionally, the proposed structure is feasible to be manufactured, which might pave the way for many novel designs of graphene-based photon detection, energy harvesting systems, and plasmonics devices.

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