Low-loss plasmonic supermodes in graphene multilayers

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Abstract: We investigate the supermodes in arbitrary layers of graphene sheets, which are collective guided modes formed by coupling of surface plasmon polaritons (SPPs) in each graphene sheet. In terms of the dispersion relation, we analyse the effective indexes and mode profiles of the supermodes. Numerical simulations reveal that the supermodes can be well approximated by linear superposition of SPPs in individual graphene sheets. Among all the possible supermodes, there is an interesting one possessing both lowest propagation loss and shortest mode wavelength. The loss of the supermode decreases as the number of layers increases and saturates at about 5 layers. The graphene multilayers may find potential applications in low-loss plasmonic waveguides and so constructed optical devices.

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OCIS codes: (240.6680) Surface plasmons; (230.4170) Multilayers; (130.2790) Guided waves.

References and links

Surface plasmon polaritons (SPPs) are electromagnetic waves guided at the interface of two materials with opposite signs of dielectric constants [1, 2]. The strong field confinement makes it possible to manipulate the light at nanoscale below the diffraction limit. They could find applications in integrated optics, transformation optics, biosensing, and solar cells [3, 4]. In the past decades tremendous interest has been focused on the metal-based plasmons [5–11]. While the intrinsic material loss at visible regime, to some degree, has hindered the practical applications of metal-based SPPs [12]. Recently, considerable attention has been paid to graphene, a one-atom-thick material with exotic electric, optical, mechanical and thermal properties [13–18]. In the THz and far-infrared regime, monolayer graphene can support transverse magnetic (TM) polarized SPPs with short wavelength and low propagation loss. The properties of graphene-based SPPs can be tuned by doping or gating, making them a promising platform for plasmonic applications [12, 16]. So far, quite a lot of works have been reported on SPPs in monolayer [19–22], double layers [23–26] and infinite layers of graphene [27]. Recently, the ultra-broadband absorber based on graphene multilayers have been
proposed [28, 29] and their transmission and phase modulation properties [30] have also been studied.

In this work, we shall investigate the supermodes in graphene multilayers composed of arbitrary layers of graphene sheets. The supermode normally refers to the eigen guided modes in composite-array waveguides, which was firstly introduced to describe the mode in phase-locked arrays of semiconductors lasers [31]. Here we borrow the concept of supermode to characterize the collective SPP mode in the graphene multilayer, which stems from the evanescent coupling of SPPs in individual graphene sheets. We firstly give an accurate algorithm based on the transfer matrix method (TMM) [30] to calculate the mode indexes and profiles of the supermodes. In order to reveal how SPPs in individual graphene are compounded to form the supermode, we also analyse the interaction between SPPs in adjacent graphene based on coupled-mode theory. There is a supermode with lower propagation loss and shorter mode wavelength compared with other possible ones. The influence of the graphene numbers and other parameters are also considered in detail.

2. Algorithm of solving the supermodes in graphene multilayers

A schematic of the graphene multilayer is shown in Fig. 1. We assume the TM polarized SPPs propagate along the z direction in each graphene sheet, then the magnetic field in the region between the \((n-1)\)th and \(n\)th graphene sheets can be written as the superposition of waves in opposite directions:

\[
H_z(x) = \begin{cases} 
A_n^+ \exp[+ik_z(x-x_n)] + A_n^- \exp[-ik_z(x-x_n)], & x_{n-1} < x < x_n \\
A_{n+1}^- \exp[-ik_z(x-x_n)] + A_{n+1}^+ \exp[+ik_z(x-x_{n+1})], & x_n < x < x_{n+1}
\end{cases}
\]

where \(k_z = (\epsilon_d k_0^2 - \beta^2)^{1/2}\) with \(k_0 = 2\pi/\lambda\) and \(\beta = n_{eff} k_0\). \(n_{eff}\) denotes the effective index of the supermode. According to Maxwell’s equations, the electric field reads

\[
E_z(x) = \begin{cases} 
-\frac{\eta_d \epsilon_z}{\epsilon_d k_0^2} \left[ A_n^+ \exp[+ik_z(x-x_n)] - A_n^- \exp[-ik_z(x-x_n)] \right], & x_{n-1} < x < x_n \\
-\frac{\eta_d \epsilon_z}{\epsilon_d k_0^2} \left[ A_{n+1}^- \exp[-ik_z(x-x_n)] - A_{n+1}^+ \exp[+ik_z(x-x_{n+1})] \right], & x_n < x < x_{n+1}
\end{cases}
\]

Considering the boundary conditions at \(n\)th graphene sheet: \(E_z(x_n) = E_z(x_n^-), H_z(x_n^-) = H_z(x_n)^+\), the field amplitudes in neighboring regions can be related with the transfer matrix
where \( \xi = \sigma_g \eta_0 / (ik_0) \), \( \kappa = k / \varepsilon_d \) and \( u = \exp(ik_d d) \). Then the transfer matrix relating the first and \((n+1)\)th dielectric regions can be written as

\[
\begin{bmatrix}
A_{n+1}^- \\
A_{n+1}^+
\end{bmatrix} = M_n \begin{bmatrix}
A_n^- \\
A_n^+
\end{bmatrix} = \begin{bmatrix}
1/2 & 1/(2\kappa) \\
1/(2u) & -1/(2\kappa u)
\end{bmatrix} \begin{bmatrix}
(1-i\xi\kappa)u & 1+i\xi\kappa \\
\kappa u & -\kappa
\end{bmatrix} \begin{bmatrix}
A_n^- \\
A_n^+
\end{bmatrix}
\]

(3)

For the eigen modes in the graphene multilayer, there should be \( A_1^+ = A_{N+1}^- = 0 \). Thus the dispersion relation is figured out by \( m_{22} = 0 \).

3. General properties of the supermodes

Now we investigate the general properties of supermodes in the graphene multilayer based on the TMM method. The excitation wavelength is firstly fixed at \( \lambda = 10 \mu m \) and the interlayer space \( d = 50 \text{ nm} \). The surface conductivity of graphene \( \sigma_g \) can be modeled by the Kubo formula [17]. The chemical potential of graphene is \( \mu_c = 0.15 \text{ eV} \). The relaxation time of electrons in graphene is given by \( \tau = \mu_c / (e V_F) \), where \( e \) is the electron charge, \( V_F \approx 10^6 \text{ m/s} \) is the Fermi velocity. In order to make the theoretical results accordance to experiments [32], we choose the impurity-limited DC mobility \( \mu = 10,000 \text{ cm}^2/\text{V} \text{s} \) at room temperature \( T = 300 \text{ K} \) [33], thus we have the relaxation time \( \tau = 0.15 \text{ ps} \).

The effective indexes of the possible supermodes in the graphene multilayer are shown in Fig. 2 as the total number of graphene sheets \( N \) varies. As \( N \) increases, more supermodes can be supported and the number of supermodes is always equal to that of graphene sheets. As \( N \) is fixed, one sees that the effective indexes manifests remarkable differences for different supermodes. We can label the supermodes by \( s = 1, 2, \ldots, N \), in terms of the increasing order of \( \text{Re}(n_{\text{eff}}) \). For larger \( \text{Re}(n_{\text{eff}}) \), the mode wavelength is smaller. The propagation loss is determined by \( \text{Im}(n_{\text{eff}}) \). Generally, as the mode wavelength of the supermode decreases, the propagation loss is reduced accordingly. We are interested in the supermode with the lowest propagation loss, i.e., \( s = N \). The propagation loss and mode wavelength of the supermode decrease simultaneously as \( N \) increases. They both saturate when \( N \) approaches to 5. As \( N > 5 \), the mode wavelength and propagation loss will almost not change. In contrast, the supermode with largest mode wavelength (\( s = 1 \)) has the loss increasing with the total number of graphene sheets.

The magnetic field distributions of the supermodes in graphene multilayers as \( N = 2, 3, 4, 5 \) are plotted in Fig. 3. Due to the symmetry of the structure, the mode profile also experiences certain symmetry. As shown in the figures, the mode is symmetric as \( s \) is even.

![Fig. 2. Effective indexes of the supermodes in the graphene multilayer with different number of graphene sheets. (a) real and (b) imaginary parts of the effective indexes. The red circles denote the lowest loss supermodes. The green arrows represent the increasing order of the label \( s \).](#223194 - $15.00 USD
Received 15 Sep 2014; revised 2 Oct 2014; accepted 2 Oct 2014; published 9 Oct 2014
(C) 2014 OSA
20 October 2014 | Vol. 22, No. 21 | DOI:10.1364/OE.22.025324 | OPTICS EXPRESS 25327

#223194 - $15.00 USD
Received 15 Sep 2014; revised 2 Oct 2014; accepted 2 Oct 2014; published 9 Oct 2014
(C) 2014 OSA
20 October 2014 | Vol. 22, No. 21 | DOI:10.1364/OE.22.025324 | OPTICS EXPRESS 25327
and anti-symmetric as \( s \) is odd. Since there are surface currents in graphene, the magnetic field is discontinuous at the positions where graphene sheets are placed. As the supermodes are formed by the coupling of SPP mode in individual graphene sheets, the ways of coupling largely determine the mode profiles of the supermodes. As \( s = 1 \) for any \( N \), the mode is formed by the in-phase coupling of the SPPs in individual graphene sheets. In contrast, the supermode \( s = N \) is formed by the out-of-phase coupling of SPPs. The in-phase coupling results in constructive interference of the field between adjacent graphene sheets and the field enhancement, while the out-of-phase coupling leads to destructive interference and field weakening. As the surface power loss density can be written as 

\[
P_\Omega = \text{Re}(\sigma_g)|E_z|^2
\]

the in-phase coupling will yield higher propagation loss. Consequently, the supermode \( s = 1 \) undergoes the highest propagation loss and \( s = 5 \) the lowest. Note that the SPP mode in single-layer graphene is anti-symmetric with respect to the magnetic field, the supermode is anti-symmetric for in-phase coupling. For out-of-phase coupling, the magnetic field of the supermode is symmetric as \( s \) is even and anti-symmetric as \( s \) is odd.

![Fig. 3. Normalized transverse magnetic field distributions of the supermodes in the graphene multilayers.](image)

(a) \( s=1 \)  
(b) \( s=2 \)  
(c) \( s=3 \)  
(d) \( s=4 \) 

Fig. 3. Normalized transverse magnetic field distributions of the supermodes in the graphene multilayers. (a)-(d) Mode profiles of the supermodes as \( N = 2, 3, 4, 5 \) respectively. The red dashed lines represent the position of graphene. The green circles indicate the numerical results based on the FDFD computation.

4. Forming mechanisms of the supermodes

By using the coupled-mode theory, we can obtain the weight of each SPP mode of single-layer graphene in forming the supermode. As the coupling of SPPs between graphene is weak, the magnetic field of the supermodes \( H_x(x,z) \) can be written as

\[
H_x(x,z) = \left\{ \sum_{n=1}^{N} C_n H_{y,n}(x) \right\} \exp(i\beta z)
\]

where \( H_{y,n}(x) = \text{sgn}(x-x_n)\exp(-\kappa|x-x_n|) \) represents the transverse profile of SPP mode in the \( n \)th graphene sheet in the absence of other graphene, and \( \kappa = (k_{SP}^2 - \varepsilon_{0}k_0^2)^{1/2} \) with \( k_{SP} = \ldots \)
$k_0[\varepsilon_r-(2\varepsilon_0/\varepsilon_g)\Delta_1/2$ being the propagation constant of the SPPs in a single-layer graphene [12]. The weight factor of individual SPPs in forming the supermode is given by $C_n = \sin[n\pi(N + 1)]$, which is obtained by using the coupled-mode theory and periodic boundary conditions [34, 35]. For example, as $N = 5$, there are five possible supermodes in the graphene multilayer. For the supermode $s = 1$, we have $C = [1/2, \sqrt{3}/2, 1, \sqrt{3}/2, 1/2]$. As all the components are positive, the supermode is formed by the in-phase coupling of individual SPP modes. In contrast, we have $C = [1/2, -\sqrt{3}/2, 1, -\sqrt{3}/2, 1/2]$ for $s = 5$. Since the adjacent components have opposite signs, the supermode is formed by the out-of-phase coupling of individual SPP modes. The absolute value of $C_n$ represents the weight of the SPP modes in each graphene when forming the collective supermode.

Fig. 4. Normalized magnetic field distributions of the supermodes calculated by FDFD simulations based on coupled-mode theory. (a)-(e) The supermodes $s = 1, 2, 3, 4, 5$ as $N = 5$. The weight factor $C_n$ is on the top of the corresponding figure.

From Eq. (5), we can also find an efficient way to generate the supermodes in graphene multilayers. According to the weight factor, one can excite the SPPs in each graphene with proper amplitude and phase. Since the profile of the initial field is very close to that of the eigen supermode, the field will be steady quickly during propagation, forming corresponding supermodes in the graphene multilayer. Figure 4 illustrates the magnetic field distributions as SPPs are individually excited in each graphene of the multilayer with $N = 5$. The calculation is performed by using the finite-difference frequency-domain (FDFD) method, where graphene is equivalent to an ultrathin film with a thickness of $\Delta = 1$ nm and a bulk relative permittivity of $\varepsilon_{g,eq} = 1 + i\sigma_g\eta_0/(k_0\Delta)$ [24]. The minimum mesh size is set to be $\Delta/5$. The convergence of our results has been checked by calculating the effective index of a single-layer graphene with different equivalent thickness from 0.1 nm to 10 nm. The choice of 1 nm thickness brings about a computational error less than 2%. It keeps a fair balance between saving time and improving accuracy. The amplitude of the SPP mode in the $n$th graphene is set as $|C_n|$, and a phase difference of $\pi$ is introduced once the sign inversing emerges. If $C_n = 0$, it is not necessary to inject SPPs on that graphene sheet. The data of the lateral mode profiles (green circles) have been incorporated in Fig. 3(d). They are perfectly consistent with the rigorous results.

Recently, Alaee et al. have studied the interaction of the delocalized and localized SPPs in graphene [33], which are supported by periodic graphene ribbons and smooth graphene sheet, respectively. It is revealed that there are two kinds of coupling schemes between the delocalized and localized SPPs: the near-field coupling and far-field interference, corresponding to the behaviors in hybrid plasmonic oscillators and Fabry-Perot resonators, respectively. Within the coupling schemes defined by Alaee et al., the formation of the supermodes in our study can be explained by the near-field coupling of delocalized SPPs, since only uniform graphene sheets are considered and their interlayer space keeps in subwavelength.
5. Low-loss supermodes

The most interesting supermode is the one with lowest propagation loss ($s = N$). The magnetic field distributions of the supermodes are shown in Fig. 5 as $N = 1, 2, 3, 4, 5$. The mode wavelengths of the supermodes decrease from 144.9 nm to 125.4 nm, and the propagation lengths increase from 0.22 μm to 0.26 μm. One can see clearly the coupling ways of individual SPP modes forming the collective supermode. The SPPs in adjacent graphene sheets are always out of phase to each other. The mode profile is symmetric in the graphene pair as $N = 2$. The SPPs in each graphene contribute equally to the supermode. As $N > 3$, the amplitude of the SPPs at the center tends to be larger than that at the boundaries, reflecting the weight difference of SPPs in each graphene. The loss can be further decreased by increasing the number of graphene layers but will not change much as $N > 5$, as shown in Fig. 2(b).

![Fig. 5. Normalized magnetic field distributions of the lowest loss supermodes ($s = N$) in the graphene multilayer as $N = 1, 2, 3, 4, 5$, respectively.](image)

![Fig. 6. Mode wavelength and propagation length of lowest loss supermode ($s = N$) as $N = 1, 2, 3, 4, 5$ versus: interlayer space $d$, chemical potential $\mu_c$, and excitation wavelength $\lambda$. (a) and (b) fixed $\lambda = 10$ μm and $\mu_c = 0.15$ eV. (c) and (d) fixed $\lambda = 10$ μm and $d = 50$ nm. (e) and (f) fixed $d = 50$ nm and $\mu_c = 0.15$ eV.](image)

Now we consider the influence of other parameters. Figures 6(a) and 6(b) plot the dependence of the wavelength and propagation length of the lowest loss supermode on the interlayer space of graphene sheets, which are given by $\lambda_p = \lambda/\text{Re}(n_{eff})$ and $L_p = 1/[2\text{Im}(n_{eff})]$, respectively. As the interlayer space $d$ increases, the mode wavelength increases and saturates at the upper limit for a single-layer graphene. The propagation length experiences a maximum at around $d = 40$ nm. In our previous works [30, 36, 37], we have revealed that the strong
coupling occurs when the interlayer space is smaller than the plasmonic thickness of graphene, which equals 46 nm in the present case. As the coupled-mode theory is not valid for strong coupling, the supermode displays different properties with that for weak coupling. Figures 6(c) and 6(d) depict the influence of the chemical potential of graphene. As the chemical potential increases, the mode wavelength increases. At the same time, the propagation length increases. In Figs. 6(e) and 6(f), we change the exciting wavelength to see the variation of mode wavelength and propagation length. As the exciting wavelength increases, the mode wavelength increases and the propagation length increase as well. It should be mentioned that the graphene multilayers are remarkably different from the single-layer graphene in the parameter dependence, even for \( N = 2 \). That means the coupling between the SPPs in individual graphene sheets plays the most important role in forming the supermodes.

![Fig. 7. Influence of the parameters: \( d, \lambda, N, \mu_c \) on the FOM of lowest loss supermode (\( s = N \)).](image)

(a) The function FOM(\( d, \lambda, N \)) at fixed \( \mu_c = 0.15 \) eV. (b) The function FOM(\( d, \lambda, \mu_c \)) for fixed number of graphene sheets \( N = 5 \). (a) and (b) The dielectric medium is air (\( \epsilon_d = 1 \)). (c) and (d) The dielectric medium is KCl (\( \epsilon_d = 2.13 \)). In (b) and (d), the magnitudes of FOM for \( \mu_c = 0.15 \) eV (the lowest slice) are doubled.

To further investigate the influence of the parameters as a whole, we illustrate the figure of merit (FOM) of the supermodes, which is defined by FOM = \( L_p/\lambda_p \) [38, 39], as a function of \( d, \mu_c, N, \) and \( \lambda \) in Fig. 7. A larger FOM means a shorter mode wavelength at the cost of a lower propagation loss, indicating a better performance of a guided mode. In Fig. 7(a), the chemical potential is fixed at \( \mu_c = 0.15 \) eV, and the function FOM(\( d, \lambda, N \)) is shown. The FOM increases as \( N \) increases and as \( d \) decreases. There is an optimal wavelength at which the FOM has maximum value when \( N > 1 \). If we only consider the graphene multilayer as \( N = 5 \), the FOM depending on \( d, \lambda, \mu_c \) is illustrated in Fig. 7(b). As the chemical potential increases, the FOM increases accordingly, and larger FOM tends to appear at shorter wavelength. Within the range of the present parameters, a maximum magnitude of FOM~20 is achieved. Naturally we can assign different chemical potentials in each graphene sheet. Since both the mode wavelength and propagation length experience a monotone dependence on the chemical potential, the graphene sheets with identical chemical potential are more convenient to achieve optimized FOM of the supermodes. In addition, we can also use another material as the host medium. In Fig. 7(c) and 7(d) the dielectric medium is replaced by KCl (\( \epsilon_d = 2.13 \)) [36, 40]. By comparing with Fig. 7(a) and 7(b), we find the features of the
figures don’t change much and only the magnitude of the FOM decreases slightly. It reveals that the host medium with lower refractive index will benefit the propagation of the supermodes.

6. Conclusions

In conclusion, we have investigated the plasmonic supermodes in arbitrary layers of graphene sheets. By using the TMM method, we obtained the accurate effective indexes and mode profiles of the supermodes. Based on the coupled-mode theory under weak coupling approximation, we analyse the forming mechanisms of the supermodes by the coupling of SPP modes in individual graphene sheets. The analysis also provides an approach to excite the supermodes in graphene multilayers, which is validated by using the numerical calculations of FDFD. Among all the possible supermodes, there is an interesting one possessing both lowest propagation loss and shortest mode wavelength. The propagation loss of the supermode decreases as the number of graphene sheets increases and saturates at about 5 layers. By increasing chemical potential $\mu_c$ or excitation wavelength $\lambda$, the propagation loss can be further reduced. The mode can propagate as far as ~20 mode wavelengths (FOM ~20) by optimizing the parameters. The properties of low propagation loss and short mode wavelength will make graphene multilayers find great applications in low-loss plasmonic waveguides and optical waveguide devices.

Acknowledgments

This work is supported by the 973 Program (No. 2014CB921301), the National Natural Science Foundation of China (Nos. 11304108 and 11104095), and the Specialized Research Fund for the Doctoral Program of Higher Education of China (No. 20130142120091). Numerical simulations presented in this paper were carried out by using the High Performance Computing Center experimental tested in SCT-S/CGCL (see http://grid.hust.edu.cn/hpcc).