Surface plasmon dispersion and modes on the graphene metasurface with periodical ribbon arrays

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Abstract
Graphene plasmonics on the structured metasurface demonstrate many exotic properties which can combine novel nanomaterials and well-established plasmonics, providing unique opportunities to develop a series of novel photonic, plasmonic and optoelectronic devices across a wideband spectrum. Dispersion theory and its propagating characteristics of surface plasmon polaritons (SSPs) mode along the graphene metasurface can provide a powerful guidance to design related devices and systems. In this paper, the fundamental dispersion theory and the numerical studies of graphene SSPs (GSPs) on a graphene metasurface i.e. periodical ribbon arrays which are bounded by a superstrate and substrate dielectric are presented. The dispersion expression of GSPs is deduced and revealed by a modal expansion method combined with periodical boundary conditions on the structure. According to this fully analytical dispersion expression of SSPs mode on the graphene metasurface, the dispersion characteristics, propagation loss and field profiles of SSPs mode with different graphene material parameters (e.g. graphene ribbon width and chemical potential) and bounded dielectric mediums are studied and analyzed in detail in terahertz (THz) band. Moreover, the dynamical tunable dispersion characteristics of SSPs mode on the graphene metasurface via electrostatic gating of a ground metal plate can be readily obtained by applying a graphene biased voltage model to this analytical dispersion theory. The presented studies on the dispersion theory of the graphene metasurface provide an analytical method to understand the propagation characteristics of SSPs mode on the structure. Besides, the calculation results on the structure can also be used to design some novel graphene-based optoelectronic and plasmonic devices with planar gradient-index distributions such as couplers, tunable focused lens and enhanced radiation sources in THz band.

1. Introduction
Graphene is a two-dimensional (2D) carbon atoms sheet which is arranged as a planar honeycomb lattice, has displayed many exotic electric, magnetic, mechanical and thermal characteristics. Specifically, surface plasmon polaritons (SSPs) on the graphene material which is formed by the coupling of free charged carriers with incident electromagnetic field have been intensively pursued and investigated from visible to low frequency band such as terahertz (THz) spectrum [1, 2]. Graphene SSPs (GSPs) demonstrate many superior properties compared with that on the conventional metal-dielectric SSPs mode such as lower Ohmic losses and the versatile tunable capabilities. In this context, SSPs mode on the graphene material is responsible and promising to develop a new class of optoelectronic, photonic and plasmonic devices and systems across a wide spectrum band.

Graphene is usually viewed as an infinite 2D monolayer material without closed edge. However, recent studies show that graphene sheet with specific structured surfaces (i.e. graphene metamaterial or metasurface) provide a new platform to study GSPs [3–13]. SSPs mode on the graphene corrugated surfaces is similar to the conventional 2D metamaterial with tailored electromagnetic properties. A plethora of graphene metasurfaces with patterned shapes have been proposed and studied, such as graphene ribbons [3, 4], graphene ring [5], 'U'-
shaped corrugated graphene structure [7], cross-shaped [8], elliptical shape [9], graphene split ring [10], ‘H’-shaped graphene [11], graphene circle ring [12], sinusoidal shaped graphene structure [13] and something others like this. Besides, these periodical micro- and nano-meter shaped graphene structures reveal a much richer resonant transmission pictures and a much tighter field concentration of SSPs mode compared with un-patterned structure. Actually, the electrodynamic features have been largely modified with specific edge of graphene sheet, like the well-known armchair and zigzag-shaped edge in graphene nano-ribbon. However, most studies are focused on micrometer graphene structures and the edge SSPs mode can be reasonably ignored especially in lower THz band [3]. As a simple and specific form of graphene metasurface, periodical ribbon arrays have received enormous attentions and have been proposed for many interesting applications [14–21]. Its transmission spectrum and resonance effect have been investigated numerically and experimentally in [4, 14, 19]. The exotic properties of SSPs mode on the periodical graphene ribbon arrays are also utilized to develop some functional devices such as perfect absorber [15], polarizer converter [17], plasmonic waveguide [19], THz radiation source [21]. The plasma frequency and dispersion band in the structure is usually predicted by a scaling law which is approximately from the infinite graphene sheet [4, 14, 18]. However, a rigorous dispersion theory of SSPs mode with periodical graphene metasurface can provide more details to understand the related physical phenomena and provide a guidance to design some devices. Reference [20] presents the studies of dispersion mode on the periodical nanoribbon arrays by an ab initio time-dependent density functional theory. However, this calculation process is complicated and the analytical dispersion expression is not revealed therein.

The dispersion expression of GSPs mode on the conventional un-patterned graphene sheet with infinite boundary is well established and used for many applications. The detailed studies of dispersion theory of GSPs on the periodical graphene metasurface especially the tunable dispersion via a simply analytical expression have not been performed so far. In this paper, the general dispersion theory about GSPs mode on the periodical ribbon arrays which is bounded by a superstrate and substrate dielectric medium by a modal expansion method is presented. By solving Maxwell’s equations in different regions which is separated by periodical graphene ribbon arrays using infinite boundary conditions, the electromagnetic fields can be obtained in each region. According to the periodical impedance boundary conditions in the graphene interface using these electromagnetic field expressions, the propagating GSPs dispersion mode can then be acquired after some tedious calculations. Following this closed analytical result, the propagation characteristics include dispersion lines, damping loss and field profiles of SSP mode with different graphene material and structural parameters are studied and analyzed in THz band. Especially, the tunable dispersion characteristics via a biased drive voltage connected with a conducted metal plate are also demonstrated and calculated analytically.

2. Dispersion theory on the graphene metasurface

In this section, we first present the dispersion theory of SSPs mode on a graphene metasurface which is bounded by a superstrate and substrate dielectric medium as shown in figure 1(a). The dielectric permittivity of superstrate and substrate is \( \varepsilon_s \) and \( \varepsilon_v \), respectively. Here, graphene metasurface is periodical ribbon arrays on the \( x-y \) plane with \( z = 0 \) in the coordinate. The parameters of the patterned graphene ribbon arrays are width \( d \), period \( p \) and side length \( w \). Considering the propagating SSPs mode along \( x \) direction is a quasi-2D surface mode as studied in [12–15], the side length \( w \) of graphene ribbon is assumed infinite thus the transverse effect is
ignored. The theoretical model of tunable GSPs propagation dispersion characteristic by a gated voltage of \( V_b \) with a grounded metal plate is schematically given in figure 1(b).

Graphene can support both transverse magnetic (TM) and transverse electric (TE) SSPs mode along propagation direction which is dependent on the imaginary part of graphene conductivity [21–23]. The dispersion expression for both TM and TE SSPs mode with graphene sheet on the dielectric medium are revealed and analyzed in THz band [22]. Here, we solve the electromagnetic fields and using the graphene impedance boundary conditions for the periodical ribbon arrays in figure 1(a). In the following studies, SSPs mode is assumed as a TM mode for the application of enhanced THz radiation source with gradient-index structure by using its strong axial electric field [21]. The depth of superstrate and substrate dielectric is assumed as infinite in its semi-plane. The field components can be solved in different regions which is separated by graphene metasurface sheet on \( z = 0 \) plane. For the region above graphene metasurface \( (z > 0) \), the axial electric and transverse magnetic fields can be obtained according to Maxwell’s equations and the infinite boundary conditions, that is:

\[
E^u_n = \sum_{n=-\infty}^{\infty} A_n e^{-\gamma_n x} e^{-j\beta_n z} \\
H^u_n = \sum_{n=-\infty}^{\infty} B_n e^{-\gamma_n x} e^{-j\beta_n z}
\]

Also, for the fields under graphene metasurface \( (z < 0) \), the components are:

\[
E^l_n = \sum_{n=-\infty}^{\infty} B_n e^{-\gamma_n x} e^{-j\beta_n z} \\
H^l_n = \sum_{n=-\infty}^{\infty} -A_n e^{-\gamma_n x} e^{-j\beta_n z}
\]

In above expressions, the Bloch harmonic waves are considered for the periodical boundary conditions which are different from that in the uniform graphene sheet [22–26]. The superscript 'u' and 'l' means field components in superstrate and substrate dielectric medium, respectively. \( A_n \) and \( B_n \) are corresponding unknown index. \( \beta_n = \beta_0 + 2n\pi/p \) \((n = 0, \pm 1, \pm 2, \pm 3 \ldots)\) is propagation constant of its harmonic wave of GSPs mode. \( \gamma_n^2 = \beta_n^2 - \varepsilon_n k^2 \) and \( \tau_n^2 = \beta_n^2 - \varepsilon_i k^2 \) is transverse propagation constant in each region of \( z > 0 \) and \( z < 0 \), respectively. \( k = \omega/c \) is wave vector in vacuum, \( j \) is imaginary unit.

Next, using the boundary conditions on the graphene metasurface of \( z = 0 \), i.e.:

\[
E^u_n = E^l_n \\
H^u_n - H^l_n = \sigma_m E^u_n
\]

It should be noted that in the boundary condition of (6), graphene conductivity \( \sigma_m \) is periodical along \( x \) direction. So, its distribution is as followings:

\[
\sigma_m = \begin{cases} 
0, & mp + d < x < mp + p \\
\sigma, & mp < x < mp + d
\end{cases}
\]

Where \( \sigma \) is graphene conductivity as widely used as large area sheet [22–26]. By using above boundary conditions, the transverse magnetic field in (6) should be integrated in one period for the field discontinuity. The dispersion expression can be obtained immediately after tedious calculations by eliminating above unknown indexes. The final result of dispersion expression for GSPs mode on the graphene metasurface is:

\[
\sum_{n=-\infty}^{\infty} \frac{j\omega\varepsilon_n}{\tau_n} + \sum_{n=-\infty}^{\infty} \frac{j\omega\varepsilon_n}{\tau_n} = \frac{d}{p} \sum_{n=-\infty}^{\infty} \frac{Sa\left(\frac{\beta_n p}{2}\right)}{Sa\left(\frac{\beta_n d}{2}\right)} \sigma
\]

Where \( Sa \) is sinc function as defined by \( \text{sinc}(x) = \sin(x)/x \). As predicted, GSPs mode on the graphene metasurface is closely dependent on bounded dielectric medium, graphene structure parameters and graphene conductivity. The calculation process is simplified compared with some other calculation method in [20]. Besides, the final result is fully analytical with a simple expression. The propagation characteristics of GSPs mode can be determined if graphene conductivity and graphene structural parameters are given. Thus, the presented results are very helpful to analyze some complicated graphene metasurface and lay the foundations for many interesting applications such as some passive gradient-index plasmonic devices and enhanced active THz electronic radiation source [21].
Where represented by its intraband conductivity the following studies and analysis, the frequency is in THz band thus the graphene conductivity can be represented by its intraband conductivity [21–24]. The well-known intraband conductivity is given as:

\[
\sigma_{\text{intra}}(\omega) = \frac{e^2}{\pi \hbar^2} \frac{2\kappa_0 T}{\tau - j\omega} \ln \left[ 2 \cosh \left( \frac{\mu_c}{2\kappa_0 T} \right) \right]
\]  

(9)

Where \( \omega = 2\pi f \) is radian frequency, \( e, \hbar \) and \( \kappa_0 \) are electron charge value, reduced Planck’s constant and Boltzmann constant, respectively. Graphene parameters include chemical potential or Fermi level \( \mu_c \), relaxation time \( \tau \) \( (\tau^{-1} \) is scatter rate) and temperature \( T \). For the following studies and analysis, the frequency is in THz band thus the graphene conductivity can be represented by its intraband conductivity [21–24]. The well-known intraband conductivity is given as:

3. Results and discussions

Based on above calculations, the general dispersion theory of GSPs mode is revealed for periodical ribbon arrays. In this part, we will study its propagation characteristics of GSPs mode along graphene metasurface in detail. For the following studies and analysis, the frequency is in THz band thus the graphene conductivity can be represented by its intraband conductivity [21–24]. The well-known intraband conductivity is given as:

\[
\sigma_{\text{intra}}(\omega) = \frac{e^2}{\pi \hbar^2} \frac{2\kappa_0 T}{\tau - j\omega} \ln \left[ 2 \cosh \left( \frac{\mu_c}{2\kappa_0 T} \right) \right]
\]  

(9)

where \( \omega = 2\pi f \) is radian frequency, \( e, \hbar \) and \( \kappa_0 \) are electron charge value, reduced Planck’s constant and Boltzmann constant, respectively. Graphene parameters include chemical potential or Fermi level \( \mu_c \), relaxation time \( \tau \) \( (\tau^{-1} \) is scatter rate) and temperature \( T \). For the following studies, \( \mu_c = 0.1 \text{ eV}, \tau = 0.5 \text{ ps} \) and \( T = 300 \text{ K} \) are kept constant if not mentioned additionally. Because the graphene conductivity is complex, dispersion expression (8) includes dispersion line and propagation loss with its imaginary part and real part of \( \sigma \), respectively. By substituting graphene conductivity (9) into expression (8), the dispersion lines and propagation loss can be obtained. The results with various graphene ribbon width \( \alpha \) are presented in figures 2(a) and (b). In the calculations, superstrate and substrate dielectric is assumed as isotropic silica with \( \varepsilon_{\text{in}} = \varepsilon_{\text{s}} = 3.92 \) [20–22]. Graphene ribbon arrangement period is \( p = 1.0 \mu \text{m} \). Here, graphene is assumed as infinite thin sheet and the imaginary part of conductivity is positive for the studies of TM mode. In [23], the TE SSPs mode with graphene sheet is also studied in THz band with external incident magnetic field. GSPs mode with complete graphene sheet of \( \alpha = 1.0 \) is also plotted in figure 2 as black lines. We can note that GSPs dispersion line shifts lower with decreased graphene ribbon width. This also implies that the dispersion line momentum mismatch with light line is enlarged. The real part of conductivity is negative for the studies of TM mode. In figure 2(b), the propagation losses increase along with decreased graphene ribbon width. In [22], it is shown that graphene-based TE SSPs mode exhibits a better field confinement but with a larger loss in THz regime with complete graphene sheet. Thus, the propagation loss of SSPs mode with graphene metasurface and metal–dielectric SSPs mode should be compared carefully in the future.

According to above studies, GSPs mode on the graphene metasurface demonstrates better field confinement compared with that on un-patterned sheet [22–24]. Figure 3 gives the field patterns of graphene SSPs mode (2 THz) with various graphene metasurface of \( \alpha = 0.2, 0.4, 0.6 \) and 1.0. The field patterns of GSPs mode decays exponentially into both upper and lower interface with deep sub-wavelength field confinement. The extreme sub-wavelength field confinement can open up many exciting applications such as miniature photonic circuits, plasmonic waveguide and compact photo-electronic amplifiers. It is observable that transverse field concentrates deeper on the interface with \( \alpha = 0.2 \) compared with that with uniform graphene sheet with \( \alpha = 1.0 \). This is consistent with previous studies and analysis in the dispersion band diagram.

In the above studies, the upper and lower dielectric medium is the same and is also assumed as isotropic. Reference [24] studied the plasmon waves along graphene sheet bounded with anisotropic dielectrics and long-range plasmon mode with a limited graphene thickness is studied. We here consider GSPs mode dispersion...
characteristics with different upper and lower bounded dielectric mediums. Figure 4 presents the results of dispersion lines and the propagation losses of GSPs mode with different bounded superstrate dielectric of air ($\varepsilon_u = 1$), polymethylpentene (TPX) ($\varepsilon_u = 2.1$), silica ($\varepsilon_u = 3.92$) and silicon ($\varepsilon_u = 11.7$). For single bounded graphene metasurface with $\varepsilon_u = 1$, the dispersion line of GSPs mode demonstrates larger pass-band. With increased dielectric permittivity, the dispersion band shift lower and induce a relatively larger propagation losses. For the field confinement of GSPs mode with different bounded medium as depicted in figure 5, we can note that the sub-wavelength field confinement becomes better with increased dielectric permittivity. The substrate dielectric medium is kept as the same as silica of $\varepsilon_s = 3.92$ and the superstrate medium is changed. Graphene metasurface is $d/p = 0.8$. The above studies indicate that the bounded dielectric medium can influence the propagation characteristics of GSPs mode on the structured graphene metasurfaces.

According to our dispersion theory of GSPs mode on the graphene metasurface, the propagation characteristics can also be tuned by graphene chemical potential. The fascinating properties of graphene material lie in its dynamic tunable properties via various external approaches such as chemical doping [20, 21], magnetic field [23], electrostatic gating [27], ultraviolet illuminations [28], etc. Here, we demonstrate the dynamic tunable dispersion characteristic of GSPs mode by electrostatic gating of biased voltage $V_b$, as shown in figure 1(b). Here, the tunable properties of each graphene ribbon are changed uniformly with the biased voltage. Each graphene ribbon can also be tuned individually with different graphene ribbon width and/or individual biased gate [27]. According to expression (8) and (9), dispersion lines and propagation losses can be obtained with various chemical potential $\mu_c$. The calculation results are given in figure 6 and graphene metasurface is $d/p = 0.5$. Superstrate and substrate dielectric medium is silica. We can note that the dispersion band of GSPs mode shifts lower with decreased chemical potential from 0.5 eV to 0.1 eV monotonously. The graphene conductivity increases with the chemical potential according to expression (9), leading to the propagating GSPs mode pass band enlarged based on the presented dispersion theory. This is caused by larger carrier concentration with heavy doping in the graphene material of higher level, thus the plasma frequency of GSPs dispersion mode increases. In some studies with a non-constant scattering model in graphene conductivity, larger chemical potential inversely leads to reduced graphene conductivity [29]. Figure 6(b) implies that the

![Figure 3. Field patterns of propagating GSPs mode on x-z plane with various graphene metasurface structures of d/p = 0.2, 0.4, 0.6 and 1.0. Useful graphene parameters includes chemical potential $\mu_c = 0.1$ eV and relaxation time $\tau = 0.5$ ps (In room temperature $T = 300$ K). The frequency is at 2 THz.](image-url)
propagation loss of GSPs mode can be largely decreased along graphene metasurface by heavily doping. Finally, we establish the tunable dispersion characteristics of GSPs mode on the graphene metasurface by biased drive voltage in figure 1(b). The trace of chemical potential along with a biased voltage can be defined as following expression according to [21], i.e.:
\[ \mu_c = \hbar v_F \sqrt{\pi \eta (V_b - V_{\text{Dirac}})} \] (10)

Where \( \hbar \) is reduced Planck’s constant, \( v_F = 0.9 \times 10^6 \text{ m s}^{-1} \) is Fermi velocity of Dirac fermions in graphene. \( \eta \) is constant which can be estimated from a capacitor model \([21]\), \( \eta = 9 \times 10^{16} \text{ m}^{-2} \text{ V}^{-1} \) is used in the calculation. \( V_b \) is applied biased voltage in figure 1(b) and \( V_{\text{Dirac}} \) is ideal Fermi level and is assumed as \( V_{\text{Dirac}} = 0 \) here. Thus, according to expression (8)–(10), the dispersion characteristics of GSPs mode can be obtained immediately. The results of GSPs dispersion diagram with different biased voltage are plotted in figure 7. We can note that propagation characteristic can be significantly tuned by the external biased voltage. The dynamic tunable propagation velocity can open many interesting applications such as tunable SSPs excitation source which is induced by injected electron beam. The exact synchronization of phase velocity between GSPs mode and electron beam can influence the output performance therein \([21]\).

4. Conclusions

In summary, the general dispersion theory of GSPs mode along graphene metasurface sandwiched by a superstrate and substrate dielectric medium is presented. Analytic dispersion expression of GSPs mode is revealed by solving electromagnetic fields combined with periodical boundary conditions on graphene...
metasurface. The propagation dispersion, damping losses and field profiles are also studied and analyzed with various graphene parameters and bounded dielectric mediums in THz band based on this analytical dispersion theory. The presented theories can also be applied to study other graphene metasurface with complicated surfaces. Also, the propagation characteristic of periodical graphene nano-ribbon metasurface can also be solved if the interband and intraband graphene conductivity are applied simultaneously. The dispersion theory of GSPs mode provide an useful analytic tool to study graphene metasurface and the calculation results of GSPs mode here can also be used to design and develop various novel passive and active graphene plasmonic devices like gradient-index coupler, tunable focusing lens and phase deflectors in THz band.

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