Graphene-based polaritonic crystal

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It is shown that monolayer graphene deposited on a spatially-periodic gate behaves as a polaritonic crystal. Its band structure depending on the applied gate voltage is studied. The scattering of electromagnetic radiation from such a crystal is presented calculated and analyzed in terms of Fano-type resonances between the reflected continuum and plasmon-polariton modes forming narrow bands.

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Coupling of light to the surface charges at a metal-dielectric interface gives rise to a special kind of evanescent electromagnetic (EM) waves called surface plasmon-polaritons (SPPs) [1]. The specific properties of SPPs allow for their use in a variety of practical applications. The sensitivity of SPPs to the properties of the dielectric, the metal and the interface is used in SPP-based sensors [2,3] and in high-resolution imaging [4–6]. Surface plasmons give rise to very large EM fields at the surface, which is important for surface-enhanced optical spectroscopies [7]. Moreover, the SPP wavelength can be much smaller than the photon wavelength, opening the possibility for further miniaturization of photonics components, a new field of research called nanoplasmonics [8]. Of particular interest is the ability to tune SPP modes in plasmonic devices by external control: using an electric field in a liquid crystal [9], a magnetic field in a magneto-optically active substrate [10], thermal heating [11], or a light beam focused on a non-linear coating [12].

The possibility of tuning the amount of free carriers in graphene using an external gate allows for an effective control of the material’s optical properties [13–16]. Exploring graphene, a tunable two-dimensional (2D) metal, for plasmonics at the nano-scale reveals new physical effects and opens exciting possibilities in this field [17–20]. When compared to their counterparts in conventional 2D electron systems, SPPs in graphene exhibit some new and unusual properties, such as the $1/4$-power density dependence of the SPP frequency [17] and the existence of $s$-polarized waves [18]. Moreover, SPPs in graphene can potentially be used in a variety of practical applications. For example, using the amplification of SPPs in graphene opens the possibility to create a terahertz radiation source [21]; employing the attenuated total reflection (ATR) configuration with a gated graphene layer allows for a resonant switching of the reflection coefficient of an external EM wave from nearly unity to almost zero [22].

Recently, a new class of metamaterials based on SPPs in graphene, either deposited on a periodically corrugated surface [23] or composed of an array of micro-ribbons [24] was proposed, with a high potential interest for transformation optics. When SPPs propagate along a periodically modulated surface, the concept of a "surface polaritonic crystal" can be introduced [5], where the SPP dispersion shows a band-gap structure [25], in analogy with a photonic crystal. In this Letter we propose and theoretically analyze a new type of SPP crystal, based on a graphene sheet deposited on top of a periodically modulated gate electrode (wafer), as schematically represented in Fig. 1(a).

In order to achieve the periodic modulation of graphene’s conductivity, we consider a single graphene layer in the plane...
We assume that the prism occupies the half-space \(d < x < 0\), where \(d\) is the modulation depth and \(g = 2\pi/D\). A conductive wafer is placed over this modulated surface, serving as a gate contact. If a constant gate voltage \(V\) is applied between the graphene plane and the wafer, a periodic modulation of the graphene conductivity can be achieved. If \(D \gg h(x)\), the carrier density in graphene can be expressed as \(n(x) = \varepsilon_2 \varepsilon_F/4\pi e^2 h(x)\), where \(e\) is the electron charge and \(\varepsilon_2\) is a coefficient between 1 and 2 depending on the charge distribution on the corrugated gate electrode (further in the Letter we use \(\varepsilon_2 = 1\)). Owing to the periodicity of the surface relief, the carrier density in graphene is a periodic function with the same period \(D\), thus resulting in the periodicity of its optical conductivity, \(\sigma(x, \omega) = \sigma(x + D, \omega)\). The latter can be related to the local value of the chemical potential counted with respect to the Dirac point, \(\mu(x) = h v_F \{\pi n(x)\}^{1/2}\), where \(v_F\) is the Fermi velocity.

As it is shown below, the periodic modulation of the optical conductivity leads to the possibility of direct coupling of a propagating EM wave to the surface plasmons (Fig. 1(a), left, where \(\varepsilon_2\) is the dielectric constant of the medium above graphene). However, only those SPP modes which lie within the light cone, \(\omega/k = c/\sqrt{\varepsilon_2}\), shown by dash-dotted lines in Fig. 1(b), can be excited this way. In general, for the SPP excitation one has to consider an ATR structure like the one described in Ref. [22] which includes a prism with a dielectric constant \(\varepsilon_3\) (Fig. 1(a), right). Usually there is a gap between the graphene sheet and the prism, which we shall model as a dielectric layer of a thickness \(d\) and a dielectric constant \(\varepsilon_2\).

We assume that the prism occupies the half-space \(z < -d\) and a \(p\)-polarized EM wave impinges on the boundary \(z = -d\), coming from \(z = -\infty\) at an angle of incidence \(\Theta\).

Since the dielectric properties of the structure are periodic along \(x\), the solution of Maxwell’s equations, \(\text{rot} \mathbf{E}^{(m)} = \mu \mathbf{H}^{(m)}\), \(\text{rot} \mathbf{H}^{(m)} = -i\varepsilon m \mathbf{E}^{(m)}\) for the \(p\)-polarized wave [with components \(\mathbf{E} = (E_x, 0, E_z)\) and \(\mathbf{H} = (0, H_y, 0)\)] can be written as Fourier-Floquet series:

\[
H_y^{(m)}(x, z) = \sum_{n=-\infty}^{\infty} A_n^{(m)} \exp(i\kappa_n z) + B_n^{(m)} \exp(-i\kappa_n z),
\]

\[
E_x^{(m)}(x, z) = \sum_{n=-\infty}^{\infty} \frac{q_n^{(m)}}{i\varepsilon m} \left[ A_n^{(m)} \exp(i\kappa_n z) - B_n^{(m)} \exp(-i\kappa_n z) \right],
\]

where \(Q_{n,l}^{(m)} = 1/2 \left[ Q_{n,l}^{(1,+)} - Q_{n,l}^{(1,-)} \right]\), \(Q_{n,l}^{(1,\ell)} = 1/2 \left[ Q_{n,l}^{(1,+)} + Q_{n,l}^{(1,-)} \right]\), and \(Q_{n,l}^{(2,+)} = 1/2 \left[ Q_{n,l}^{(2,+)} + Q_{n,l}^{(2,-)} \right]\) for different \(n\). (1) and (2) can be either propagating (with \(\kappa > 0\)) or evanescent (with \(\kappa < 0\)) modes which lie within the light cone. The latter can be related to the periodicity of its optical conductivity, \(\sigma(x, \omega) = \sigma(x + D, \omega)\). The latter can be related to the local value of the chemical potential counted with respect to the Dirac point, \(\mu(x) = h v_F \{\pi n(x)\}^{1/2}\), where \(v_F\) is the Fermi velocity.

The meaning of the coefficients \(A_n^{(m)}, B_n^{(m)}\) is different for the different media. The waves corresponding to the different terms in Eqs. (1) and (2) can be either propagating (with \(\Im(q_n^{(m)}) < 0\)) or evanescent (with \(\Re(q_n^{(m)}) > 0\)). Since the incident wave in the medium 3 possesses only the \(n = 0\) component (zero harmonic), \(\Im(q_n^{(3)}) < 0\) and the coefficients \(B_0^{(3)} = \delta_{n,0} H_1 \exp(-i\kappa_0 d)\) are proportional to the magnetic field amplitude \(H_1\) in the incident wave. In the medium 1, the coefficients \(A_0^{(1)} = 0\) correspond to the absence of the corresponding harmonics coming from \(z = 0\). Then, multiplying the matrices \(M^{1+2} M^{2+3}\), and taking into account the block-diagonal structure of the matrix \(M^{2+3}\), after some algebra we obtain the following equations for the amplitudes of the reflected harmonics, \(r_n = A_n^{(m)} \exp(-i\kappa_n d)\):

\[
\hat{R} \times (\ldots, r_n, r_{n+1}, \ldots)^T = (\ldots, H_n^1, H_{n+1}^1, \ldots)^T,
\]
where the elements of the matrix $\hat{R}$ and the vector $H_n^i$ are

$$R_{n,n'} = \left[ \delta_{n,n'} F_0^{(1)} - \frac{4\pi n_0^{(2)} \sigma_{n,n'}}{i e \varepsilon_2} \right] \left[ S_{n'} + F_n^{(2)} C_{n'} \right] + \delta_{n,n'} \left[ C_{n'} + F_n^{(2)} S_{n'} \right]$$

$$H_n^i = \left\{ \delta_{n,0} F_0^{(1)} - \frac{4\pi n_0^{(2)} \sigma_{n}}{i e \varepsilon_2} \right\} \left[ S_0 - F_0^{(2)} C_0 \right] + \delta_{n,0} \left[ C_0 + F_0^{(2)} S_0 \right] \right\} H(k)$$

with $C_n = \cosh(\kappa g_0^{(2)} d)$ and $S_n = \sinh(\kappa g_0^{(2)} d)$. In order to obtain the general properties of SPPs in graphene with periodically modulated conductivity, we first consider the eigenvalue problem for the matrix $\hat{R}$ leading to the dispersion relation for SPPs in a flat 2D graphene layer placed between two lossless dielectric media ($\varepsilon_1$ and $\varepsilon_2$). We put $\varepsilon_1 = \varepsilon_2$ and solve the equation $\det(\hat{R}) = 0$. It yields complex eigenvalues because the graphene conductivity $\sigma(x, \omega)$ has both real and imaginary parts, therefore the SPP eigenmodes are dissipative. The SPP dispersion curve for the real part of the frequency eigenvalue, $\omega'$, vs wavenumber for the first Brillouin zone, $k \in [-g/2, g/2]$, is presented in Fig. 1(b). The imaginary part of the frequency (mode damping) is an order of magnitude smaller than $\omega'$. As it can be seen from Fig. 1(b), the SPP dispersion curve is periodic in the $k$-space, with the period $g$. There are bands of allowed SPP frequencies, separated by gaps opening at the edges and in the center of the Brillouin zone, where SPPs do not exist. As expected, the widths of the gaps increase with the increase of the modulation depth $a$ [Fig. 1(c)]. A natural question arises: is it possible to control dynamically the gap widths through some nondestructive external knob? The positive answer to this question is evident from Fig. 1(d). Since the chemical potential of graphene can be tuned by the gate voltage, one can shift the spectral position and width of the gaps by changing $V$. Therefore, the SPP crystal band structure can be controlled dynamically.

Another feature of the SPP spectrum in periodically modulated graphene is that the "scan line", $k = \kappa \sqrt{\varepsilon_2} \sin \Theta$, located within the dash-dotted lines in Fig. 1(b) crosses the SPP dispersion curves. This situation is completely different from the case of uniform graphene ([22]), where both phase and group velocities of SPPs are smaller than the velocities of light in the surrounding dielectrics. SPPs in periodically modulated graphene can be excited by an external propagating EM wave, without an ATR prism. This is illustrated by Fig. 2 where the amplitudes of the reflected field harmonics are presented; they have been calculated by solving Eq. 5 for $d = 0$ and $\varepsilon_1 = \varepsilon_2$ (in this case, $\omega$ is real).

At normal incidence ($\Theta = 0$), the zero harmonic reflection coefficient of the SPP crystal exhibits just one maximum at $\omega \approx 10$ meV [see Figs. 2(a) and (b)], which approximately corresponds to the upper edge of the second gap in Fig. 1(b). This is related to the parity of the SPP mode with respect to $x = 0$, since it is excited by a plane wave and $h(x)$ is an even function. Also from Fig. 2(b) it is clearly seen that the enhanced reflection of the zero harmonic corresponds to the excitation of the SPP harmonics with $n = -1$ and $n = 1$. They correspond to the bottom of the third allowed SPP band and, for normal incidence, are mixed into the $k = 0$ band bottom mode. For oblique incidence [Figs. 2(e)-2(f)], there are two resonances corresponding to the second and third SPP bands and producing reflected field harmonics with $n = \pm 1$. SPPs are effectively excited when the frequency and the in-plane component of the wave vector of the incident EM wave match those of SPP eigenmodes of the modulated graphene. The energy of the incident wave is transferred into the SPP harmonics with $n = \pm 1$, while the reflected wave in the far field contains only zero harmonic. Note that the position and the amplitude of the resonances can be controlled by changing the gate voltage [Figs. 2(e) and 2(f)]. Quite interestingly, the direct excitation of $n = \pm 2$ and higher SPP bands can produce propagating EM waves with $|k \pm g| \leq \kappa \sqrt{\varepsilon_2}$, scattered at angles

$$\Theta_{\pm 1} = \arcsin \left( \frac{k \pm g}{\kappa \sqrt{\varepsilon_2}} \right).$$

Let us focus on the characteristic spectral dispersion of the
The reflectivity spectrum ($R$) decreases with the increase of the incidence angle. When the Brewster angle is close to the Brewster angle, the SPP Bragg mode of the polaritonic crystal couples between the continuum of propagating EM modes in the polaritonic crystal band structure comprised between the dashed light lines in Fig. 1(b). Beyond this, one has to use the ATR scheme where SPPs are excited by an evanescent wave with a sufficiently large wavenumber, $k = k_0 \sin \Theta$. The results calculated for the ATR structure are presented in Fig. 3, where the SPP excitation conditions correspond to a minimum of the zero harmonic reflectance related to the gap between the first and the second SPP bands. The mode anticrossing, corresponding to the edges of the gap, is clearly seen in Figs. 3(a) and 3(b) (near $\Theta \approx 50^\circ$, see insets). Comparison of Figs. 3(a) and 3(b) shows that increasing the gate voltage results in an increase of the gap width, as it could be anticipated from Fig. 1(d).

To conclude, we have demonstrated that a single graphene layer deposited on a “sandwich”-like structure with a periodically corrugated gate electrode has the properties of a polaritonic crystal, namely, possesses a band structure with gaps that can be tuned by the gate voltage. This crystal exhibits Fano-type resonances in the reflectance of incident EM waves due to the excitation of plasmon-polariton Bragg modes.

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