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Published in: Optics Letters

DOI: 10.1364/OL.40.002076

Publication date: 2015

Document Version: Final published version

TE-polarized graphene modes sustained by photonic crystal structures

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Received March 9, 2015; accepted April 1, 2015; posted April 8, 2015 (Doc. ID 235727); published April 29, 2015

We present the design of a supporting photonic crystal structure that would allow for the excitation of the predicted transverse electric (TE) polarized plasmon-polaritons (TE-SPPs) in single and multi-layer graphene at cryogenic temperatures and room temperature, respectively. The graphene conductivity can then be calculated as

\[ \sigma = \sigma_0 + \sigma' + i\sigma'' \]

with \( \sigma_0 = \sigma_0/(\epsilon\epsilon_0) = 2.3 \times 10^{-2} \), the effective index \( n_{\text{eff}} = k_s/\lambda_0/(2\pi) \) real and \( k_s \) the wave number of the TE-SPP projected on \( \hat{z} \) (see Fig. 1). Since TE-SPPs are propagating along the graphene sheet, i.e., the fields must be evanescent in the substrate and cladding, we have \( n_{\text{eff}} > n_1 \geq n_0 \), and \( s'' < 0 \). To find out how large a \( s'' \) is required for a certain asymmetry, we take the lower limit for \( n_{\text{eff}} \), namely \( n_{\text{eff}} = n_1 \) in Eq. (1), so that we obtain

\[ s''n_0^2 > n_1^2 + n_0^2 (\approx 2(n_1 - n_0) \text{ if } n_1 - n_0 \text{ small and } n_0 \approx 1). \]

Let us now consider the scenario of a graphene sheet with a chemical potential of \( \mu = 0.5 \text{ eV} \). Choosing a...
wavelength in the region where the TE-SPPs can propagate [5], \( \lambda_0 = 1.31 \, \mu \text{m} \), we obtain a value of \( \sigma = (0.310 - i0.457) \lambda_0 \) at room temperature \((T = 300 \, \text{K})\). Neglecting \( s' \), the largest possible refractive index difference that is able to sustain TE-SPPs in the graphene sheet is given by \( n_3 - n_0 = 0.10 s_0^5 = 5.5 \times 10^{-3} \). It is assuredly impossible to find a solid substrate material with a refractive index \( n_1 \) that is close to \( n_0 \). Including the loss term \( s' \) will even further lower the maximally allowed asymmetry between the cladding and substrate.

A way to solve this problem is to use a terminated PC designed so that its optical response “mimics” that of the cladding around the excitation wavelength of the TE-SPP. Such a strategy, which has already been employed for detecting long-range surface plasmons in thin metal films [10], yields the desired effective symmetry required to sustain TE-SPPs. The latter can then be detected by exciting the structure with light at a tuneable wavelength or tunable incident angle through a substrate underneath the PC (see Fig. 1), and measuring the dips in the reflection spectrum.

We again consider the single sheet of graphene described above, for which the TE-SPP has a complex effective index of \( n_{\text{eff}}^g = n_0 + (0.7 + i1.9) \times 10^{-3} \). As shown in Fig. 1, we consider placing the graphene sheet on a (finite) PC with unit cells consisting of 2 different layers with thicknesses \( d_a \) and \( d_b \) and refractive indices \( n_a \) and \( n_b \), made of SiO\(_2\) and TiO\(_2\), respectively, a commonly used combination for the design of optical filters [11]; we imagine placing the PC structure on top of a SiO\(_2\) substrate.

Next, we use a T-matrix algorithm for the multilayer [12] and the graphene sheet [13], together with the values for \( n_a \) and \( n_b \) given in [14], to calculate the values of \( d_a \) and \( d_b \) where both the optical symmetry that the TE-SPP experiences and the coupling toward the TE-SPP of light incident from the substrate are maximized around \( \Re\{n_{\text{eff}}^g\} = n_0 + 0.7 \times 10^{-3} \), corresponding to an angle of incidence in the substrate of \( \theta = \sin^{-1}(\Re\{n_{\text{eff}}^g\}/n_0) = 43.7389^\circ \approx 43.74^\circ \), where \( n_0 \) is the refractive index of the substrate. We note that the two conditions cannot both be perfectly satisfied due to the finiteness of the PC and the influence of the substrate [6], so we calculate \( d_a \) and \( d_b \) using numerical optimization such that an optimal balance between the two conditions is attained.

We will discuss more advanced design strategies in more detail in a future publication. For a PC with 5 unit cells \( (N_{\text{per}} = 5) \), we arrive at \( d_a = 212.0 \, \text{nm} \) and \( d_b = 206.1 \, \text{nm} \).

We now plot the reflectivity of light incident from the substrate, \( |R_{N1}|^2 \), in Fig. 2 as a function of the incident angle at the fixed wavelength of \( \lambda_0 = 1.31 \, \mu \text{m} \) in the cases where the graphene sheet is absent or present on the designed PC. We observe a dip in \( |R_{N1}|^2 \) (in the region of \( \theta \) where total internal reflection (TIR) takes place between the substrate and cladding) when the graphene sheet is present, contrary to the case where the graphene sheet is absent. From the inset in Fig. 2, we can observe that the reflectivity minimum at \( \theta_{\text{min}} \) nicely overlaps with the angle where the excitation of the TE-SPP is expected, \( \theta^g \), showing that the device’s operation is indeed optimized around \( \Re\{n_{\text{eff}}^g\} \). Further calculations have revealed that an equivalent way to detect the TE-SPP is to consider the \( |R_{N1}|^2 \) spectrum as a function of the wavelength at the fixed angle \( \theta_{\text{min}} \approx 43.74^\circ \) (rather than performing an angular sweep at fixed wavelength) and observe the reflection dip induced by the graphene sheet at the design wavelength of \( \lambda_0 = 1.31 \, \mu \text{m} \).

Despite the agreement of \( \theta_{\text{min}} \) with \( \theta^g \), one can question whether the excitation observed should be associated with a TE-SPP. After all, terminated PC structures are able to sustain Bloch surface waves (BSWs), i.e., surface excitations that can exist even without graphene coverage [15]. There is only one reflection dip visible in the spectrum of Fig. 2, indicating only one excitation is present. Yet if the graphene sheet were removed from right above the PC and put far above it, we would naturally expect that the system would possess two essentially uncoupled excitations: a BSW associated with the PC (as we will see below) and a TE-SPP associated with the graphene. When the graphene is right above the PC, how should the one surviving excitation indicated by the dip in Fig. 2 be understood?

To address this issue we calculate the dispersion relations (or \((E, k_x)\)-diagrams), with \( E = \hbar c/\lambda_0 \) the photon energy) of the optical modes that occur for different distances between the graphene sheet and the PC structure. To be sure our results are not affected by loss mechanisms and to obtain an exact solution for real \( k_x \), we consider an infinite PC such that we avoid radiation

![Fig. 1. Proposed PC-based experimental setup to measure the TE-SPPs in a single layer of graphene.](image-url)

![Fig. 2. \( |R_{N1}|^2 \) as a function of the incident angle \( \theta \) for the setup without graphene coverage (dotted lines) and with graphene coverage (full lines). The blue and red colors indicate the absence or the presence of an additional PMMA layer, respectively. The inset also indicates the angles \( \theta_{\text{TIR}} \) and \( \theta^g \approx \theta_{\text{min}} \).](image-url)
losses in the substrate, and neglect the graphene loss by setting \( s' = 0 \) for each value of \( E \). In this lossless case, some parameters will slightly change compared to the previous section: for fixed \( d_a = 212.0 \, \text{nm} \), \( n_a^0 \), and \( d_b \), the number of guided modes \( n_{\text{g,eff}} \) and \( d_b = 206.0 \, \text{nm} \), respectively.

In Fig. 3, we plot the dispersion relations that result as we decrease the distance \( d_{\text{air}} \) between the graphene sheet and the terminated PC structure from infinity to zero. At an infinite separation, there is indeed both a BSW associated with the terminated PC structure (its dispersion relation \( E_{\text{BSW}}(k_x) \) shown by the red line), and the TE-SPP associated with the graphene (its dispersion relation \( E_g(k_x) \) shown by the grey line). For \( d_{\text{air}} \) finite but large—see the curves for \( d_{\text{air}} = 120 \, \mu\text{m} \) in Fig. 3—we see the first signs of coupling between these excitations, breaking the degeneracy where \( E_{\text{BSW}}(k_x) \) and \( E_g(k_x) \) cross (at the red dot \((E, \nu)_{\text{cross}}\)) and producing upper and lower dispersion relations that we label \( E_{g,\text{PC}}(k_x) \) and \( E_{g,\text{PC}}'(k_x) \), respectively. The splitting between these dispersion relations increases as \( d_{\text{air}} \) decreases; in Fig. 3 we also plot the results for \( d_{\text{air}} = 45 \, \mu\text{m} \), where \( E_{g,\text{PC}}'(k_x) \) is approaching the light line \( E_{\text{air}} \) shown by the black line. While \( E_{g,\text{PC}}(k_x) \) survives as \( d_{\text{air}} \to 0 \), \( E_{g,\text{PC}}'(k_x) \) vanishes into the air light line for \( d_{\text{air}} < 38 \, \mu\text{m} \) in the range of \((E, \nu)\) values considered in Fig. 3.

This clarifies why at \( d_{\text{air}} = 0 \, \mu\text{m} \) (Fig. 2) there is only one dip; there is only one surviving dispersion relation, and only one excitation. The dip corresponds to the blue dot in Fig. 2 labeled \((E, \nu)_{\text{design}}\). What is the nature of the excitation here? Certainly it can be understood as one point on the \( E_{g,\text{PC}} \) line for \( d_{\text{air}} = 0 \, \mu\text{m} \), which takes the nature of a shifted BSW dispersion relation (compare the red curve). Yet, the excitation at \((E, \nu)_{\text{design}}\) exists on all of the lower dispersion relations \( E_{g,\text{PC}}(k_x) \), independent of the distance \( d_{\text{air}} \) between the graphene sheet and the terminated PC. This is of course because \((E, \nu)_{\text{design}}\) is our design point, where the terminated PC mimics the air cladding in its optical response such that it makes no difference what the value of \( d_{\text{air}} \) is. Furthermore, the excitation at \((E, \nu)_{\text{design}}\) survives in the presence of the graphene and the absence of the terminated PC, but not vice versa. So while it is certainly correct to identify the excitation at \((E, \nu)_{\text{design}}\) as one point on a shifted BSW dispersion relation, it is also correct to identify it as a TE-SPP guided by the graphene, but sustained by the PC.

To illustrate this, we show the field profiles at the design point \((E, \nu)_{\text{design}}\) for \( d_{\text{air}} = 0 \, \mu\text{m} \) and \( d_{\text{air}} = 5 \, \mu\text{m} \) in Figs. 4(a) and 4(b) respectively. Note that in both cases, the maximum field is located at the graphene sheet. Certainly in Fig. 4(b) it is natural to identify the excitation as a graphene TE-SPP with the PC underneath, and indeed no less so in Fig. 4(a). The decay of the envelope field in the PC indicates bandgap operation, equivalent with the field decay in the cladding. Further calculations have revealed that these observations are also true for the field distributions in the finite cladding structure including the graphene loss, corresponding to the reflection dip in Fig. 2, which only explore a region of \((E, \nu)\) space close to \((E, \nu)_{\text{design}}\). In this region of parameter space, we argue it makes physical sense to associate the excitation as a graphene TE-SPP.

Yet the TE-SPP excitations lie extremely close to the light line of air, where total internal reflection (TIR) takes place between substrate and cladding. This means that the unavoidable surface roughness in fabricated samples of the PC would make the detection of the TE-SPPs difficult. Even if we assume that an experiment would not be affected by this problem, observing the reflectivity dip—or finding the angle where the dip takes place in case \(|R_{\text{N1}}|^2 \) is measured as a function of wavelength—would require a very high angular resolution, due to the fact that the dip is extremely narrow (in the order of 0.0001°–0.001°).

**Fig. 3.** Dispersion relations \( E_{g,\text{PC}} \) (blue) and \( E_{g,\text{PC}}' \) (green) for air gap thicknesses of \( d_{\text{air}} = 120 \, \mu\text{m} \), \( d_{\text{air}} = 45 \, \mu\text{m} \) and \( d_{\text{air}} = 0 \, \mu\text{m} \). \( E_{g,\text{PC}} \) does not exist at \( d_{\text{air}} = 0 \, \mu\text{m} \) for the considered set of \((E, \nu)\)-values. The light line of air, \( E_{\text{air}} \) (black), and the excitations in the bare PC and the isolated graphene, \( E_{\text{BSW}} \) (red) and \( E_g \) (gray), respectively, together with the design and crossing points \((E, \nu)_{\text{design}} \) (blue dot) and \((E, \nu)_{\text{cross}} \) (red dot), respectively, are also indicated. All the data is plotted relative to \( E_{\text{air}} \) and \( k_x_{\text{design}} \).

**Fig. 4.** Normalized field profile of the \( E_{g,\text{PC}} \) (blue) at \((E, \nu)_{\text{design}}\) when (a) \( d_{\text{air}} = 0 \, \mu\text{m} \) and (b) \( d_{\text{air}} = 5 \, \mu\text{m} \). (c) Normalized field profile of the TE-SPP (blue) in the finite structure covered with a 100-nm-thick layer of PMMA, corresponding to the reflectivity dip in Fig. 2. The red lines indicate the normalized field profiles of the excitations in the corresponding symmetric structures. The light-gray and dark-gray regions in (a)-(b)-(c) correspond to the layers with refractive indices \( n_g \) and \( n_b \), respectively, while the blue region in (c) corresponds to the PMMA layer.
These issues can be overcome by depositing an extra dielectric layer, such as PMMA, on top of the graphene. As an illustration, we imagine a 100 nm-thick layer of PMMA (refractive index taken to be \( n_g = 1.481 \)) on top of the graphene. The mode in the corresponding symmetric structure (a graphene sheet with on both sides the PMMA layer) has an \( \Re(n_{eff}) \) of \( n_0 + 0.116 \). To achieve the required “optical” symmetry in this case, we match the reflectivities of the PC and the PMMA layer at this \( \Re(n_{eff}) \) and end up with \( d_g = 226.3 \) nm and \( d_b = 219.9 \) nm if we maximize the coupling as well. We then recalculate the \(|R_N|\) spectra and plot the results together with the other spectra in Fig. 2. Figure 2 clearly shows that the dip, and the associated excitation, is shifted to higher \( \theta \)-values, further away from \( \theta^{(\text{IR})} \), such that the optical response of this new configuration would be far less affected by the surface roughness. In addition, we see that the dip is much wider and can therefore be located more easily during the measurements. We also evaluate the influence of the scattering losses (from the interface roughness of the PC layers) on the structures’ optical response using the strategy described in [17]. These calculations have revealed that the scattering induces only a small dip in the reflection spectra when no graphene is present and that the dips in the reflection spectra from Fig. 2—although slightly more shallow—do not shift when the scattering losses are included in the calculations. As such, the scattering losses do not affect the detection of the TE-SPP.

Finally, we see from Fig. 4(c) that at the reflection dip, the maximum of the field is located at the graphene sheet—as was true for the excitation in the finite structure without PMMA coverage, evaluated previously—and neither in the PC top layer nor in the PMMA layer. In analogy with the simpler structure, this indicates that the observed excitation here can be considered as the TE-SPP of a graphene sheet bounded by PMMA, but with a PC below the graphene that optically mimics the PMMA layer.

In conclusion, we have shown that at a particular wave number the excitation in a graphene sheet bounded by a cladding above and a properly designed PC below can be thought of as a graphene TE-SPP sustained by a PC that optically mimics the cladding; the graphene sheet experiences a “symmetric environment”. In fact, this holds within a neighborhood of this particular wavenumber, as we will discuss in a future publication. We have also shown that depositing an extra dielectric layer such as PMMA on top of the structure will shift the TE-SPP sufficiently far from the TIR line so that several parasitic effects should not be problematic, thus enabling for the first time the excitation of the TE-SPPs at room temperature even in nonideal circumstances.

Our work reported in this Letter was in part supported by the Research Foundation—Flanders (FWO - Vlaanderen) that provides an Aspirant grant for I. Degli-Eredi and a Postdoctoraal Onderzoeker grant for N. Vermeulen, in part by the EU-FET grant GRAPHENICS (618086), the ERC-FP7/2007-2013 grant 336940, IAP Belspo (IAP P7-35), VUB-Methusalem, VUB-OZR, and in part by the National Sciences and Engineering Research Council of Canada.

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