Tunable surface waves at the interface separating different graphene-dielectric composite hyperbolic metamaterials

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Abstract: Despite the fact that metal is the most common conducting constituent element in the fabrication of metamaterials, one of the advantages of graphene over metal is that its conductivity can be controlled by the Fermi energy. Here, we theoretically investigate multilayer structures comprising alternating graphene and dielectric layers as a class of hyperbolic metamaterials for THz frequencies based on a general simple model of the graphene and the dielectric layers. By employing a method of matching the tangential components of the electrical and magnetic fields, we derive the relevant dispersion relations and demonstrate that tuning can be achieved by modifying the Fermi energy. Moreover, tunability of the graphene-dielectric heterostructures can be enhanced further by changing either the thickness of the dielectric layers or the number of graphene sheets employed. Calculated dispersion relations, propagation lengths of plasmon modes in the system are presented. This allows us to characterize and categorize the modes into two groups: Fermel-Berreman modes and surface plasmon polaritons.

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References and links

Particularly hyperbolic metamaterials (HMs) [1–5], which are a subcategory of uniaxially anisotropic materials have in recent years captured intensive attention of researchers. Graphene sheets, separated by dielectric layers, can be considered as a composite material with uniaxial electric properties. Graphene layers allow to control the complex effective permittivity of the composite for electric field components polarized parallel to the graphene sheets. Some interesting electromagnetic properties offered by such uniaxial anisotropic materials have in recent years captured intensive attention of researchers. Particularly hyperbolic metamaterials (HMs) [1–5], which are a subcategory of uniaxially anisotropic materials, possessing a number of advantages, have been in the center of attention. For instance, it has been concluded that the properties of negative refraction and
subwavelength imaging can take place in the anisotropic media with lower losses leading to an easier fabrication process [1]. Very dramatic manifestations are demonstrated by the optical topological transitions recently discovered in electromagnetic metamaterials, as these optical effects are not subject to the restrictions of the Fermi exclusion principle [2]. It should be mentioned, that HMs open wide avenues for researchers providing possibilities for metamaterials at mid-infrared frequencies since highly doped semiconductor materials behave like metals (i.e. have a large negative real part of the permittivity) so that HMs can be fabricated using alternating layers of doped and undoped semiconductor materials [4]. Furthermore, HMs have been theoretically predicted as electromagnetic absorbers for scattered fields. This was experimentally demonstrated by placing scatters on top of HM, showing enhanced absorption but it was neither perfect nor narrow-band absorption [5]. Indeed, the isofrequency wavevector dispersion in an uniaxially anisotropic medium can be elliptic for some polarization, and under certain conditions a hyperbolic relation which leads to many interesting physical properties can evolve [6,7]. In case of a hyperbolic dispersion, ideally, the waves can propagate and carry power over a wide spatial spectrum as opposed to a finite propagating spectrum in common (elliptic) media. Considerable attention which has been focused on the study of hyperbolic media and hyperbolic metamaterials in recent years is largely due to their relatively simple geometry yet many interesting properties, such as high density of states, all-angle negative refraction and hyperlens imaging beyond the diffraction limit [7,8].

This paper investigates a multilayer HM design based on a graphene-dielectric composite heterostructure [9–13]. Not surprisingly, a significant amount of recent works is dedicated to studying graphene as a building block in hybrid metamaterial designs [10]. Recent studies have shown a novel class of HMs where metallic layers are substituted by graphene sheets [11]. The HM based on a semi-infinite stack of graphene-dielectric multilayers is discussed in a topical work [12]. The analysis was performed at a temperature of 4 K, thus neglecting the graphene losses and dealing with purely real permittivity and wavenumbers. Herein, graphene is realized as a two-dimensional honeycomb structure with a thickness of a monolayer of carbon atoms, and is a type of gapless semiconductor [14,15]. A recent work in [16] discussed surface waves between graphene-based HM and isotropic media, thus dealing with the interface separating anisotropic media and a dielectric. Here we focus on an interface between two different anisotropic media. Moreover, the novelty of the present study lies in the fact that analytic formulas that express the dispersion relations have been derived. These are general and are applicable to multilayer structures comprising alternating graphene and dielectric layers. These yield correct results for known analytic solutions [17] and in some cases offers an attractive method of finding a solution without necessity of time consuming numerical methods. Additionally, we demonstrate that one can tune the frequency range of surface waves by varying the Fermi energy of graphene sheets. Also, we show that it can be controlled by modifying the thickness of the dielectric in the graphene-dielectric structure or the number of layers of graphene sheets. The accuracy of the surface modes is verified fulfilling a comparison with an exact numerical solution following which we consider the stability of the surface modes. The numerical procedures have been fulfilled by satisfying the boundary conditions at a planar interface of two anisotropic media.

**Tunable hyperbolic metamaterial made of graphene-dielectric multilayers**

Let us consider a hyperbolic metamaterial heterostructure consisting of stacked graphene sheets separated by dielectric layers, as shown schematically in Fig. 1.
Fig. 1. Schematic view of an interface separating two different infinite layered nanostructured metamaterials formed by alternating graphene and dielectric layers. Herein, indexes “1, 2” correspond to the graphene and dielectric layers correspondingly.

To describe the optical response of such a system, we apply the effective-medium approach which is justified if the wavelength of the radiation considered is much larger than the thickness of any layer. It is based on averaging the structure parameters. Hence, further in this paper we consider the effective homogeneous media for two semi-infinite periodic structures. The effective permittivities are as follows [18]:

\[
\begin{align*}
\epsilon'_1 &= \frac{\epsilon_1 d_1 + \epsilon_2 d_2}{d_1 + d_2} \\
\epsilon''_1 &= \frac{\epsilon_1 d_1 + \epsilon_2 d_2}{d_1 + d_2} \\
\epsilon'_I &= \frac{\epsilon_1 \epsilon_2 (d_1 + d_2)}{\epsilon_1 d_1 + \epsilon_2 d_2}, \\
\epsilon''_I &= \frac{\epsilon_1 \epsilon_2 (d_1 + d_2)}{\epsilon_1 d_1 + \epsilon_2 d_2},
\end{align*}
\]

where subindices I and II refer to the first and second (top and bottom) metamaterial under consideration, respectively. Matching the tangential components of the electrical and magnetic fields at the interface implies the dispersion relation for the surface modes localized at the boundary separating two anisotropic media [19]. We assume the permittivities \(\epsilon_{1,3}(\omega)\) to be frequency dependent as the corresponding layers are represented by graphene.

Within the random-phase approximation and without an external magnetic field, graphene may be regarded as isotropic and the surface conductivity can be written as follows [20,21],

\[
\sigma = i\epsilon_0 \mu / \pi h^2 (\omega + i / \tau),
\]

where \(\omega, h, e, \mu, \tau\) is the frequency, Planck constant, charge of an electron, chemical potential (Fermi energy), and phenomenological scattering rate, respectively. The Fermi energy \(\mu\) can be straightforwardly obtained from the carrier density \(n_{2D}\) in a graphene sheet,

\[
\mu = h v_F \sqrt{\pi n_{2D}},
\]

where \(v_F\) is the Fermi velocity of electrons. It should be mentioned, one can electrically control the carrier density \(n_{2D}\) by an applied gate voltage, thus
leading to a voltage-controlled Fermi energy $\mu$ [16]. Here we assumed that the electronic band structure of a graphene sheet is unaffected by the neighboring layers. Thus, the effective permittivity $\varepsilon_g$ of graphene can be calculated as follows [22]:

$$
\varepsilon_g = 1 + i \sigma / \varepsilon_0 \omega d_g,
$$

where $d_g$ is the thickness of graphene sheet, $\varepsilon_0$ is the permittivity in the vacuum.

It should be mentioned, that the frequency range of the surface wave existence could be dramatically controlled by modifying the permittivities and thicknesses of the layers [17] employed in the HMs. One needs to evaluate the tangential components of the electric and magnetic fields at the interface and obtain a single surface mode with the propagation constant seeking to get the unique dispersion relation for the surface modes confined at the interface between two metamaterials [19].

$$
\beta = k \sqrt{\frac{(\varepsilon_1^\mu - \varepsilon_1^\sigma)}{\varepsilon_1^\mu - \varepsilon_1^\sigma}},
$$

where $k$ is the absolute value of wavevector in vacuum and $\beta$ is the component of the wavevector parallel to the interface. It is interesting to notice that in the case $\varepsilon_1 = \varepsilon_3$, $\varepsilon_2 = \varepsilon_4$, $d_1 \neq d_2 \neq d_3 \neq d_4$, the obtained result for the dispersion is as follows:

$$
\beta = k \sqrt{\frac{\varepsilon_1^\mu (d_1 \varepsilon_1^\mu + i \sigma) \left( d_1 \varepsilon_1^\mu + d_2 \varepsilon_1^\mu + i \sigma \right)}{d_1^2 \varepsilon_1^\mu \varepsilon_3^\mu \omega^2 + 2 d_1^2 \varepsilon_1^\sigma \varepsilon_3^\sigma \omega^2}},
$$

while the dispersion for the case of $\varepsilon_1 = \varepsilon_3$ and $\varepsilon_2 \neq \varepsilon_4$, $d_1 \neq d_2 \neq d_3 \neq d_4$ is as follows:

$$
\beta = k \sqrt{\frac{\varepsilon_2 \varepsilon_4 (d_1 + d_2) (d_3 + d_4) \varepsilon_3^2 \left( \frac{d_2 \varepsilon_2 + d_3 \varepsilon_2 + d_4 \varepsilon_4}{d_1 + d_2} - \frac{d_3 \varepsilon_3 + d_4 \varepsilon_3}{d_1 + d_2} \right)}{d_1 \varepsilon_2 + d_2 \varepsilon_2 - d_3 \varepsilon_3 - d_4 \varepsilon_3}}.
$$

In case of $\varepsilon_1 = \varepsilon_3$ and $\varepsilon_2 \neq \varepsilon_4$, $d_1 = d_3$, $d_4 = d_2$

$$
\beta = k \sqrt{\varepsilon_3^\mu \varepsilon_3^\mu (d_1 + d_2) (d_2 \varepsilon_2 + \sigma \varepsilon_2) \left( \sigma^2 - D - C - B + d_1 \varepsilon_1^\mu \varepsilon_3 \omega^2 - A + d_2 \varepsilon_2 \varepsilon_3 \omega^2 \right)^2 + d_1^2 \varepsilon_1^\mu \varepsilon_3 \omega^2}.
$$

where $A = d_1^2 \varepsilon_1^\mu \varepsilon_3 \omega^2$, $B = d_1 d_2 \varepsilon_1^\mu \varepsilon_3 \omega^3$, $C = d_2 d_3 \varepsilon_2 \varepsilon_3 \omega^2$, $D = d_1^2 \varepsilon_1^\mu \varepsilon_3 \omega^2$.

A clear understanding of the wave propagation depends on a grasp of the propagation length denoted as the distance the wave travels along the interface until the energy has been reduced to $e^{-1}$ of its original value. As the energy is proportional to the square of the field ($\text{energy} \sim |H|^2 \sim e^{-2\text{Im}(\beta)}$), the propagation length is [23,24]:

$$
L_p = \frac{1}{2 \text{Im}(\beta)}
$$

Engineered effective permittivity of graphene based HMs

Figures 2 (a)-2(c), 3(a)-3(c) show the permittivity spectra for the perpendicular components of the multilayer heterostructure under consideration (Fig. 1). According to [25], all structures containing one or more interfaces can be qualitatively considered as a hyperbolic layer. A proper selection of parameters allows access to the epsilon-near-zero regime [26].
It is possible to electrically control the frequency of the hyperbolic dispersion curve by applying a gate voltage on the graphene sheet, which is demonstrated in Figs. 2(a), 3(a), 4(a), 5(a). At this point, we assume that the temperature is $T = 300\text{K}$, and the other parameters are $d_g = 0.35\text{nm}$, $\tau = 0.5\text{ps}$. PbS is selected as the dielectric layer with relative permittivity $\varepsilon_d = 18.8$ and slab thickness $t_d = 10\text{ nm}$. It is clear that one has the potential to achieve the resonant behavior of $\varepsilon_\perp$ by varying the Fermi energy; moreover, the increase of the Fermi energy causes a tuning of the resonant frequencies over the higher frequency range. Therefore, our graphene-based layered structure has the potential to serve as the building block for various HM-based optical devices.

Fig. 2. The influence of (a), Fermi energy $\mu$, (b) thickness of dielectric $d_d$, and (c), number of graphene sheets $N$ on the real part of $\varepsilon_\perp$. $N = 1$, $d_d = 10\text{ nm}$ in (a), $N = 1$, $\mu = 0.5\text{eV}$ in (b), and $d_d = 10$, $\mu = 0.5\text{eV}$ in (b).

Fig. 3. The influence of (a), Fermi energy $\mu$, (b) thickness of dielectric $d_d$, and (c), number of graphene sheets $N$ on the imaginary part of $\varepsilon_\perp$. $N = 1$, $d_d = 10\text{ nm}$ in (a), $N = 1$, $\mu = 0.5\text{eV}$ in (b), and $d_d = 10$, $\mu = 0.5\text{eV}$ in (b).
Based on Figs. 2-5, one can conclude that \( \varepsilon \)-near-zero (ENZ) and \( \varepsilon \)-near-pole (ENP) regimes are not coincidently located in the same spectral position in case of the current structure under consideration.

In addition to the Fermi energy, the resonant behavior of \( \varepsilon_{\perp} \) depends on the fill factors of the dielectric and graphene sheet, as shown in Figs. 2(b) and 3(b). From Fig. 2(b), we can...
clearly distinguish the shift of the resonant frequency of $\varepsilon_{\perp}$ to the higher frequencies as the thickness $d_d$ is increased. Aside from the thickness of dielectric $d_d$, the thickness of the graphene sheets also play great role in the behavior of $\varepsilon_{\perp}$, as shown in Figs. 2(c), 3(c). At this point we deal with the controlled thickness of graphene influenced by the number of layers of graphene sheets $N$, i.e. $d_g = N d_d$. It can be observed that the resonant frequency shifts to higher frequencies quickly as the number of layers $N$ is decreased.

The dispersion relations

In this section we preset dispersion curves computed after performing the homogenization of two HMs. Thus, in Fig. 6 the dispersion curves for the case $\varepsilon_1 = \varepsilon_3$, $\varepsilon_2 = \varepsilon_4$ and $d_1 \neq d_3 \neq d_2 \neq d_4$ are reported. The dispersion curves of spoof SPPs at the boundary of two metamaterials with $d_1 = 0.35\text{nm}$, $d_2 = 10\text{nm}$, $d_3 = 0.25\text{nm}$, $d_4 = 10.1\text{nm}$ are shown in Fig. 6. Moreover, it should be mentioned, that Fig. 6 gives the dispersion of surface waves with the effective parameters shown in Figs. 2(a), 3(a), 4(a), 5(a), the blue line is the free-space light line.

![Graph showing dispersion relations](image)

Fig. 6. The dispersion of surface waves (a); propagation lengths (b) and absorption (c) at different Fermi energy, where $N=1$, $d_d=10\text{ nm}$, $\varepsilon_1 = \varepsilon_3$, $\varepsilon_2 = \varepsilon_4$ and $d_1 \neq d_3 \neq d_2 \neq d_4$ and the blue line in (a) is the free-space light line.

The frequency ranges of surface wave can be tuned by changing the Fermi energy, which is consistent with the dependence of the $\varepsilon_{\perp}$ on the Fermi energy as shown in Fig. 2 (a). It should be mentioned that decreases in the Fermi energy $\mu$ will move the dispersion curves to lower frequencies; in contrast, increases in the Fermi energy $\mu$ move them to higher frequencies. As seen from Fig. 6, the smallest asymptotic frequency is achieved by employing the smallest Fermi energy. The former tunability property suggests that the surface wave can be engineered by the Fermi energy of the graphene sheets. It should be mentioned, that SPP excitations match the part of the dispersion curves lying to the right of the light line due to their bound nature. Consequently, special phase-matching techniques such as a grating or
prism coupling [27], nearfield excitation [28], and end-fire coupling [29] are required for their excitation via three-dimensional beams [30]. Between the regime of the bound and radiative modes, a frequency gap region with purely imaginary $\beta$ prohibiting propagation exists.

As the graphene is not modeled as lossless, $\beta$ is complex, leading to a finite propagation length (Eq. (4)), drawn in Fig. 6(b).

Turning now to the second case under in our study, i.e. $\varepsilon_1 = \varepsilon_3$, $\varepsilon_2 = \varepsilon_4$ and $d_1 \neq d_2 \neq d_3 \neq d_4$, in Fig. 7 four modes are represented at the boundary of two different metamaterials with $\varepsilon_4 = 2.25$. As seen from Fig. 7, the smallest asymptotic frequency corresponds to the case $\mu = 0.5$ eV. Compared with the dispersion relation of depicted in Fig. 6, it can be seen that the bound SPPs approach now a maximum, finite wave vector at the surface plasmon frequency of the system. Also, the quasi-bound [31], leaky part of the dispersion relation is allowed due to the fact, that $\text{Re}(\beta)\neq 0$. Thus $\beta$ does not tend to infinity as the surface plasmon frequency is approached, but folds back and eventually crosses the light line.

Fig. 7. The dispersion of surface waves (a); propagation lengths (b) and absorption (c) at different Fermi energy, where $N=1$, $d_2=10$ nm, $\varepsilon_1 = \varepsilon_3$, $\varepsilon_2 = \varepsilon_4$ and $d_1 \neq d_2 \neq d_3 \neq d_4$ and the blue line in (a) is the free-space light line.
As in previous cases, the case denoted as $\varepsilon_1 = \varepsilon_3$, $\varepsilon_2 \neq \varepsilon_4$ and $d_1 = d_3$, $d_2 = d_4$ will be illustrated by means of the dispersion diagrams of the TM modes. In Fig. 8, four different modes are presented. It is of particular interest to examine the effect of controlling the fill factors of the dielectric and graphene sheet as shown in Fig. 8. First, we discuss the influence of the thickness of the dielectric $d_d$ on the dispersion curve (see Fig. 8(a)). We find that the upper limit moves to the higher frequencies as $d_d$ is increased. This is consistent with the effect of $d_d$ on the frequency range of $\varepsilon_{\perp}$. Moreover, the frequency range for surface waves can also be controlled by increasing the number of graphene layers, as shown in Fig. 8 (c). The dependence of the frequency range in which surface waves exist on the thickness of dielectric and layer number of graphene sheets provides an unprecedented degree of freedom to control the surface wave at the near-infrared frequencies.

It should be mentioned, that negative values of the electrical length and absorption in Figs. 6(b), 6(c), 7(b), 7(c), 8(b), 8(d)-8(f) which result from non-physical solutions of the dispersion equation and have been omitted in line with [32]. Moreover, the sketched graphs imply the presence of the surface waves propagating for a long distance. This is caused by the fact that the real part of $\beta$ is very low within this spectral region. It should be taken into account, that the same phenomena takes place in case of the interface separating uniaxial metamaterial and isotropic medium [33].

The imaginary parts of the wavevector (i.e. absorption) are plotted in Figs. 6(c), 7(c), 8(e), 8(f). Taking advantage of the absorption resonances, one can show that the simple multilayer structures without possessing any periodic corrugation have the prospective to act as directive and monochromatic thermal sources [34].

By presenting a modal analysis, we now show that the physical origin of the bulk absorption in metamaterials is due to the excitation of leaky bulk polaritons called Ferrel-
Berreman modes [35–37]. As a matter of fact, volume charge oscillations at the ENZ of the metal (bulk or volume plasmons) are formed by the bulk metal. The important property to note now is that these excitations are in the form of a completely longitudinal wave and hence cannot be excited with free space light (which a transverse wave). The top and bottom interface couple in case of films of metal with thicknesses less than the metal skin depth, permitting for collective charge oscillations across the film. In such a case, the bulk plasmon is no longer purely longitudinal and can interact with free space light at frequencies near the metal ENZ [38]. Ferrell addressed this approach for metallic foils in [39], Berreman - for polar dielectric films in [40]. Radiative excitations which we call FB modes are supported by the multilayer metamaterials with the employed graphene layers. It is worthwhile mentioning, that these FB modes are different from surface plasmon polaritons supported by metal foils, due to the reason that in case of surface plasmon modes, energy propagates along the surfaces of the metal, whereas in FB modes volume charge oscillations are setup across the foil and energy propagates within the bulk of the metal. The bulk polaritons under consideration have transverse wavevectors similar to free space light and exist to the left of the light line. Thus, in Figs. 6(a), 7(a), 7(c) it is interesting to observe the FB modes which exist at energies near the ENZ of the hyperbolic metamaterial to the left of the light line.

Conclusions

In conclusion, we have outlined a method to investigate the dispersion diagrams of hyperbolic metamaterials. This work aims at providing a comprehensive and updated picture suggesting a dynamic control of the hyperbolic properties, which is extremely desirable in view of device applications. In summary, a graphene-based layered structure treated as the hyperbolic metamaterial is presented. We provided the dispersion relations for various cases, and discussed the controllable properties of the effective permittivity of the graphene-based HMs. There are three important conclusions that can be drawn from results presented here (i) Compared with the dispersion relation in case of \( \varepsilon_1 = \varepsilon_3, \varepsilon_2 = \varepsilon_4 \) and \( d_1 \neq d_2 \neq d_3 \neq d_4 \) depicted in Fig. 5, the quasibound, leaky part of the dispersion relation is narrowed for the case \( \varepsilon_1 = \varepsilon_3, \varepsilon_2 \neq \varepsilon_4 \) and \( d_1 \neq d_2 \neq d_3 \neq d_4 \) (Fig. 6) (ii) the perpendicular component of effective permittivity can be tuned by changing the Fermi energy applied on the graphene sheets, the thickness of dielectric, and the number of layers of graphene sheets in HMs (iii) the frequency range of surface wave existence can be engineered by varying the Fermi energy of graphene and the fill factor of dielectric or graphene sheets in the unit cell of HMs.