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| **Author(s)** | Xiang, Yuanjiang; Guo, Jun; Dai, Xiaoyu; Wen, Shuangchun; Tang, Dingyuan |
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Engineered surface Bloch waves in graphene-based hyperbolic metamaterials

Yuanjiang Xiang,¹,²,³ Jun Guo,¹,² Xiaoyu Dai,¹,² Shuangchun Wen,² and Dingyuan Tang¹*

¹School of Electrical and Electronic Engineering, Nanyang Technological University, 639798 Singapore
²Key Laboratory for Micro-/Nano-Optoelectronic Devices of Ministry of Education, College of Physics and Microelectronic Science, Hunan University, Changsha 410082, China
³xiangyuanjiang@126.com
⁴EDYTang@ntu.edu.sg

Abstract: A kind of tunable hyperbolic metamaterial (HMM) based on the graphene-dielectric layered structure at near-infrared frequencies is presented, and the engineered surface Bloch waves between graphene-based HMM and isotropic medium are investigated. Our calculations demonstrate that the frequency and frequency range of surface Bloch waves existence can be tuned by varying the Fermi energy of graphene sheets via electrostatic biasing. Moreover, we show that the frequency range of surface Bloch waves existence can be broadened by decreasing the thickness of the dielectric in the graphene-dielectric layered structure or by increasing the layer number of graphene sheets.

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1. Introduction

Surface electromagnetic waves (SEWs) are a special type of waves that are confined at the interface between two media with different properties [1, 2]. One of the best known examples of SEWs is surface plasmon polariton (SPP), which is formed at the interfaces between metals and dielectrics [3, 4]. SPPs only exist for TM polarization and there is no surface modes exist for TE polarization. SPP has attracted a wide spread attention in the last decade mainly due to their applications in sensing, microscopy, or integrated optics [5, 6]. However, when one of the two media at the interface is periodic structures (photonic crystals or superlattices), the Bloch surface waves (BSWs) may appear at the boundary within the photonic bandgaps [7, 8]. It has also been shown that the lateral condensation of the BSWs in the waveguide is well described by the 2D Snell’s law [9]. BSWs have potential applications in optical sensing [10–12], enhancement of Goos-Hanchen shift [13], and surface-enhanced Raman spectroscopy [14]. For BSWs, the Bloch wavevector is perpendicular to the interface of the periodic structure and the dielectric layer, and hence the Bloch wavevector is not propagating along the interface. Moreover, most recently, Vukovic et al. proposed another
surface wave propagating in metal-dielectric superlattices and isotropic dielectric medium where the Bloch wavevector is parallel to the interface of the two media [15]. This surface wave has been named as **surface Bloch waves** owing to the Bloch wave propagating along the interface [15].

Hyperbolic metamaterial (HMM) is a uniaxial anisotropic medium having the hyperbolic form of the dispersion relation [16]. HMMs can be realized at optical frequencies using metal-dielectric multilayers [17, 18] or metallic nanorods/nanowires in a dielectric host [19, 20], and at terahertz and infrared frequencies using semiconductor-dielectric multilayers [21, 22]. HMM promises a variety of potential applications including negative refraction [23, 24], broadband Purcell effect [20, 25], imaging hyperlens [26, 27], optical waveguide [28, 29], and perfect thermal emitters [30].

Recently, graphene has attracted intensive scientific interest owing to its incredible physical properties showing great potential applications in nano-electronic devices and optoelectric devices with ultrahigh electron mobility, ultrafast relaxation time for photo-excited carriers, and gate variable optical conductivity [31]. Graphene plasmonics have generated great interest among scientific community because of the ability of graphene to tune the plasmon dispersion by varying the chemical potential [32]. It seems to be a good candidate for designing tunable optical device that operates in both THz and optical frequency ranges [33]. Most recently, graphene-based HMMs composed of stacked graphene sheets separated by thin dielectric layers have been proposed and investigated [34, 35], it has been demonstrated that such graphene-based HMMs can be used for the negative refraction at THz frequencies [36], the spontaneous emission enhancement [34, 35], the perfect absorption [37], tunable broadband hyperlens [38], tunable infrared waveguide [39], and so on. However, these HMMs have been realized and investigated mainly at THz frequencies, and mid- or far-infrared frequencies. Graphene-based HMMs at the near-infrared frequencies and visible light are still not demonstrated. In the present paper, we suggest a new class of tunable HMMs for near-infrared frequencies based on the graphene-dielectric layered structure, and reveal that such graphene structures can support a controllable surface Bloch wave between graphene-based HMM and isotropic medium.

![Fig. 1. (a) Scheme of the interface of the semi-infinite graphene-based hyperbolic metamaterial and the semi-infinite isotropic dielectric; (b) effective permittivity of the graphene-based layered metamaterial; (c) dispersion curve of the graphene-based hyperbolic metamaterial.](image)

**2. Graphene-based HMMs at the near-infrared frequencies**

**2.1 The optical properties of graphene sheets**

Consider the geometry shown in Fig. 1(a), where the semi-infinite periodic structure created by alternating layers of graphene and conventional dielectric is placed on the left of the homogeneous dielectric. The unit cell of the layered structure is formed by a transparent material of dielectric constant $\varepsilon_d$ and slab thickness $t_d$ and graphene sheets of surface...
conductivity $\sigma$ and slab thickness $t_g$. The period of the layered structure is $t = t_d + t_g$. Experimentally, the multilayer composed of dielectric and graphene can be prepared by the following procedures: the dielectric layer is first coated on a SiO$_2$ substrate through thermal evaporation, and then the high quality graphene sheets prepared using CVD method are coated on the top of the dielectric layer after a chemical vapor deposition, finally the multilayer is realized by stacking of many graphene/dielectric layers on the SiO$_2$ substrate. The surface conductivity of graphene is highly dependent on the working wavelength and Fermi energy. Within the random-phase approximation and without external magnetic field, the graphene is isotropic and the surface conductivity $\sigma$ can be written as a sum of the intraband $\sigma_{\text{intra}}$ and the interband term $\sigma_{\text{inter}}$ [39], where

$$\sigma_{\text{intra}} = \frac{ie^2 k_g T}{\pi \hbar^2 (\omega + i/\tau)} \left( \frac{E_F}{k_g T} + 2 \ln(e^{\frac{E_F}{k_g T}} + 1) \right), \quad \sigma_{\text{inter}} = \frac{ie^2}{4\pi \hbar} \left[ \frac{2E_F - (\omega + i\tau^{-1}) \hbar}{2E_F + (\omega + i\tau^{-1}) \hbar} \right],$$

where $\omega$ is the frequency of the incident light, $e$ and $h$ are universal constants related to the electron charge and reduced Planck’s constants, respectively. $E_F$ and $\tau$ are the Fermi energy (or chemical potential) and electron-phonon relaxation time, respectively. $k_g$ is the Boltzmann constant, and $T$ is a temperature in K. The Fermi energy $E_F$ can be straightforwardly obtained from the carrier density ($n_{2D}$) in a graphene sheet,

$$E_F = h v_F (\pi n_{2D})^{1/2}, \quad v_F = 10^6 \text{ m/s}$$

is the Fermi velocity of electrons. Here, the carrier density $n_{2D}$ can be electrically controlled by an applied gate voltage, thereby leading to a voltage-controlled Fermi energy $E_F$ and hence the voltage-controlled surface conductivity $\sigma$, this could provide an effective route to achieve electrically controlled surface Bloch wave. We assume that the electronic band structure of a graphene sheet is not affected by the neighboring graphene sheets, hence the graphene’s effective permittivity $\varepsilon_g$ be written as $\varepsilon_g = 1 + i\sigma/(\varepsilon_\infty \omega \varepsilon_g)$, where $\varepsilon_\infty$ is the permittivity in the vacuum.

### 2.2 Bulk Bloch waves of the graphene-dielectric layered structure

Assuming that the electric (magnetic) field is in the form $A \exp(ik_x z + ik_y x + ik_z y - i\omega t)$, the dispersion relation of Bloch modes in the infinite layered media is described by the two-components bulk Bloch waves,

$$\cos(k_z t_g) = \cos(k_{g,x} t_g) \cos(k_{d,x} t_d) - \frac{1}{2} \left( \frac{F_1 + F_2}{F_1} \right) \sin(k_{g,y} t_g) \sin(k_{d,y} t_d),$$ (2)

where $k_g = (\varepsilon_g k_0^2 - k_z^2)^{1/2}$, $k_d = (\varepsilon_d k_0^2 - k_z^2)^{1/2}$, $k_0 = \omega/c$, $k_z^2 = k_y^2 + k_z^2$, $F_1 = \varepsilon_g / k_g$, $F_2 = \varepsilon_d / k_d$ for p-polarized mode, and $F_1 = 1/k_g$, $F_2 = 1/k_d$ for s-polarized mode.

### 2.3 Dispersion relation of graphene-dielectric layered structure in the subwavelength limit

In the subwavelength limit, i.e., $k_{g,y} t_g << 1$ and $k_{d,y} t_d << 1$, one can expand $\cos(k_z t_g)$ and $\sin(k_z t_g)$ in a Taylor series, $\cos(k_z t_g) = 1 - (k_z t_g)^2 / 2 + O((k_z t_g)^3)$ and $\sin(k_z t_g) = k_z t_g + O((k_z t_g)^2)$. Substituting them into Eq. (2) and neglecting the high-order terms, we have the dispersion relationship simplified as
\[
\frac{\sin^2\left(\frac{k_f t}{2}\right)}{\varepsilon_\perp} + \frac{t^2 k_f^2}{4 \varepsilon_\parallel} = \frac{t^2}{4} k_0^2,
\]
for p-polarization and
\[
\frac{\sin^2\left(\frac{k_f t}{2}\right)}{\varepsilon_\perp} + \frac{t^2 k_f^2}{4 \varepsilon_\parallel} = k_0^2 \frac{t^2}{4},
\]
for s-polarization, respectively, where \( \varepsilon_\perp = f_g \varepsilon_g + \varepsilon_d \), \( \varepsilon_\parallel = \left( f_g \varepsilon_g + f_d \varepsilon_d \right)^{-1} \), \( f_g = t_g / t \) and \( f_d = t_d / t \) are the filling ratio of the graphene sheet and dielectric, respectively. Equations (3) and (4) give the dispersion relations for the bulk waves in the infinite graphene-dielectric layered metamaterial in the subwavelength limit. If we adopt additional approximation \( k_f t \ll 1 \), these equations will recover to the dispersion relations in the uniaxial crystal, \( \varepsilon_\perp^2 + k_0^2 \varepsilon_\parallel = k_0^2 \) and \( \varepsilon_\parallel^2 + k_0^2 = \varepsilon_\perp k_0^2 \), respectively.

### 2.4 Effective permittivity and hyperbolic dispersion of graphene based HMMs

As an example, in Fig. 1(b) we plot the effective permittivities \( \varepsilon_\parallel \) and \( \varepsilon_\perp \). Here, we assume that the Fermi-energy of graphene \( E_F = 0.50 \text{ eV} \), and the other parameters are \( T = 300 \text{ K} \), \( t_g = 0.35 \text{ nm} \), \( \tau = 0.5 \text{ ps} \). PbS is selected as the dielectric layer with relative permittivity \( \varepsilon_d = 18.8 \) and slab thickness \( t_d = 10 \text{ nm} \), where the absorption loss of dielectric has been neglected. It is seen from Fig. 1(b) that \( \varepsilon_\parallel \) exhibits resonant behavior and \( \varepsilon_\perp \) almost keeps constant. Moreover, Re\( (\varepsilon_\parallel) < 0 \) and Re\( (\varepsilon_\perp) > 0 \) near the wavelength of optical communication \( \lambda = 1550 \text{ nm} \), hence Eq. (6) denotes a dispersion curve of hyperboloid. Figure 1(c) illustrates this case at \( \lambda = 1550 \text{ nm} \) and 1540nm. These dispersion curves have two sheets and the wavelength range of the hyperbolic band is determined by the condition \( \varepsilon_\parallel = 0 \).

### 2.5 Engineered effective permittivity of graphene based HMMs

The wavelength of the hyperbolic dispersion curve can be electrically controlled by an applied gate voltage on the graphene sheet, which is demonstrated in Fig. 2(a). It is clear that the resonant behavior of \( \varepsilon_\parallel \) can be tuned by varying the Fermi energy \( E_F \), and the resonant wavelengths of \( \varepsilon_\parallel \) move to the shorter wavelength with the increases of Fermi energy \( E_F \). Actually, the resonant wavelength can be tuned to the visible light if we apply enough voltage to the graphene sheet. Therefore, our graphene-based layered structure has the potential to achieve various HMM-based optical devices.

In addition to the Fermi energy, the resonant behavior of \( \varepsilon_\parallel \) is dependent on the fill fractions of dielectric and graphene sheet, as shown in Figs. 2(b) and 2(c). Decrease in thickness of dielectric \( t_d \) leads to the decrease of fill factor of dielectric \( f_d \) and increase of fill factor of dielectric \( f_g \), hence the graphene sheets are getting more and more important in the HMMs. From Fig. 2(b), we find that the resonant wavelength of \( \varepsilon_\parallel \) shifts to longer wavelength as the thickness \( t_d \) is decreased, and the peak value of \( \varepsilon_\parallel \) is enhanced. Furthermore, it is important that the wavelength range of the negative \( \varepsilon_\parallel \) is also extended simultaneously. These properties are significant to control the surface Bloch wave, which will be illuminated later on. Aside from the thickness of dielectric \( t_d \), the thickness of graphene sheets also play great role in the behavior of \( \varepsilon_\parallel \), as shown in Fig. 2(c). Here the thickness of
graphene is controlled by the number of layers of graphene sheets \( N \), \( t_g' = N t_g \) and \( \sigma' = N \sigma \). It can be observed that the resonant wavelength shifts to longer wavelength quickly as the number layers \( N \) is increased, and the peak value of \( \varepsilon \) and wavelength range of negative \( \varepsilon \) are enhanced obviously.

\[
\text{Fig. 2. The influences of (a) Fermi energy } E_F, \text{ (b) thickness of dielectric } t_d, \text{ and (c) number of graphene sheets } N \text{ on the real part of } \varepsilon. \text{ Where } N = 1, t_d = 10\text{nm in (a), } N = 1, E_F = 0.50\text{eV in (b), and } t_d = 10\text{nm, } E_F = 0.50\text{eV in (c), the gray line is the free-space light line.}
\]

3. Surface Bloch waves in graphene-based hyperbolic metamaterials

3.1 The dispersion relation of the Bloch waves

Now we consider the interface between infinite graphene-dielectric layered metamaterial and isotropic medium, as shown in Fig. 1(a). We assume that the surface Bloch wave can propagate in the \( yz \)-surface, and \( \phi \) is the propagation angle with respect to the \( y \)-axis. It was shown that Dyakonov surface waves exist based on the birefringent properties of metal-dielectric layered metamaterials in the long-wavelength limit [40], in our structure, Dyakonov surface waves can also exist within an interval of propagation angles \( \phi \). However, in the present paper, for simplicity in the discussion we only consider a special case, \( \phi = \pi/2 \) for \( p \)-polarization. For \( \phi = 0 \), \( k_y = 0 \), Eq. (3) can be simplified as, \( k_x^2 + k_y^2 = \varepsilon_\| \varepsilon_{\perp} \). For \( \phi = \pi/2 \), \( k_y = 0 \), Eq. (3) can be expressed as,

\[
\sin^2 \left( k_x (t/2) \right) + \frac{t^2}{4} \frac{k_x^2}{\varepsilon_\|} = \frac{t^2}{4} \frac{k_x^2}{\varepsilon_{\perp}}. \tag{5}
\]

Equation (5) is similar to the result in metamaterial and metal-dielectric superlattices [15].

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3.2 The dispersion relation of the surface Bloch wave

Using the boundary conditions, we can obtain the dispersion relation for the surface Bloch wave,

\[
\sqrt{\frac{\varepsilon_\perp \sin^2 \left( \frac{k_z t}{2} \right)}{\varepsilon_\parallel}} - \frac{\varepsilon_\parallel k_\parallel^2}{\varepsilon_\perp} + \sqrt{\varepsilon_\perp^2 - \varepsilon_\parallel^2} = 0, \tag{6}
\]

for \( \varphi = \pi/2 \). Here, \( \varepsilon_\perp \) is the permittivity of semi-infinite dielectric. The dispersion relation Eq. (6) can be applied to the arbitrary value surface Bloch wavevector \( k_z \). In the additional approximation, \( k_z t \ll 1 \), Eq. (6) can be written as

\[
\sqrt{\varepsilon_\parallel k_z^2 / \varepsilon_\perp - \varepsilon_\parallel k_\parallel^2 / \varepsilon_\perp} + \sqrt{\varepsilon_\parallel^2 - \varepsilon_\parallel k_\parallel^2 / \varepsilon_\perp} = 0, \tag{7}
\]

which is formally analogous to the dispersion relation of the surface wave in the indefinite metamaterial. The condition for this surface wave existence is \( \varepsilon_\parallel < 0 \), which is similar to the condition by considering an interface between a dielectric and a metal. This surface wave has been termed as surface Bloch wave [15], and the properties of this surface wave will be discussed as follows.

Fig. 3. The dispersion of p-polarized surface Bloch wave at different Fermi energy, where \( N = 1, t_0 = 10\text{nm} \), and the gray line is the free-space light line.

3.3 Engineered surface Bloch waves in graphene-based HMMs and isotropic medium

We consider the waves propagating along the interface between semi-infinite graphene-based HMM and semi-infinite dielectric (vacuum) with \( \varepsilon_\perp = 1 \). Figure 3 gives the dispersion of surface Bloch wave with the effective parameters shown in Fig. 2(a), the gray line is the free-space light line. From the dispersion curve we find that the p-polarized surface Bloch wave exists near the wavelength \( \lambda = 1550\text{nm} \) where \( \varepsilon_\parallel < 0 \). Moreover, the frequency ranges of surface Bloch wave can be tuned by changing the Fermi energy, which is consistent with the dependence of the negative permittivity \( \varepsilon_\parallel \) on the Fermi energy as shown in Fig. 2(a). When we decrease the Fermi energy \( E_F \), the dispersion curve moves to the lower frequency (longer wavelength); when we increase the Fermi energy \( E_F \), the dispersion curve moves to the higher frequency (shorter wavelength). This property suggests that the surface Bloch wave can be engineered by the Fermi energy of the graphene sheets.
In Fig. 3, the frequency range for surface Bloch wave existence is narrow. However it can be extended by controlling the fill factors of the dielectric and graphene sheet in the HMMs as shown in Fig. 4. First, we discuss the influence of the thickness of dielectric $t_d$ on the dispersion curve (see Fig. 4(a)). We find that both the upper and the lower limits move to longer wavelength as $t_d$ is decreased, however the lower limit moves more quickly than the upper limit, which leads to the broader frequency range for surface Bloch wave existence. This is consistent with the effect of $t_d$ on the wavelength range of negative $\varepsilon$. The frequency range for surface Bloch wave existence can also be broadened by increasing the number of graphene layers, as shown in Fig. 4(b). The dependence of frequency range for surface Bloch wave existence on the thickness of dielectric and layer number of graphene sheets provides more degree of freedom to control the surface Bloch wave at the near-infrared frequencies.

4. Conclusions

In conclusion, we have presented a graphene-based layered structure as the hyperbolic metamaterials (HMMs) at the near-infrared frequencies. We have derived the dispersion relation for graphene-dielectric layered structure for both s- and p-polarizations in the subwavelength limit, and discussed the controllable properties of the effective permittivity of the graphene-based HMMs. It is found that the parallel components of effective permittivity is negative near the communication wavelength and it can be tuned by changing the Fermi
energy applied on the graphene sheets, the thickness of dielectric, and the layer number of graphene sheets in HMMs. We also reveal that this HMM can support p-polarized surface Bloch wave, and the frequencies and 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 HMMs.

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