Abstract This paper studies and classifies the electromagnetic regimes of multilayer graphene-dielectric artificial metamaterials in the terahertz/infrared range. The employment of such composites for waveguide-integrated modulators is analysed and three examples of novel tunable devices are presented. The first one is a modulator with excellent ON-state transmission and very high modulation depth: > 38 dB at 70 meV graphene’s electrochemical potential (Fermi energy) change. The second one is a modulator with extreme sensitivity towards graphene’s Fermi energy - a minute 1 meV variation of the latter leads to > 13.2 dB modulation depth. The third one is a tunable waveguide-based passband filter. The narrow-band cut-off conditions around the ON-state allow the latter to shift its central frequency by 1.25% per every meV graphene’s Fermi energy change.

The majority of conventional devices suitable for guiding microwaves cannot be used in the THz/IR band due to pronounced skin-effect in metals. Nevertheless, there are ways to significantly reduce the losses [11]. In particular, dielectric-lined hollow waveguides [12,13] demonstrate relatively low-loss performance and are currently considered as a solution for transferring terahertz radiation. This fact motivated us to select a hollow waveguide as a base for the proposed terahertz modulators.

Is it important to keep in mind the fact that the electromagnetic response of graphene undergoes substantial changes as one increases the frequency from microwave to optical values (Fig. 1). Graphene conductivity $\sigma$ can be analytically modeled using the Kubo formula [17, 18], which takes both the intraband and interband transitions into account:

Ultrasensitive terahertz/infrared waveguide modulators based on multilayer graphene metamaterials

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1. Introduction

Active development of terahertz (THz)/infrared (IR) science and technology has created a growing demand for new electronic and quasi-optical devices. In particular, the promising opportunities for broadband high-speed terahertz communication require new techniques for real-time manipulation of radiation. Various approaches have been proposed for THz/IR waves amplitude, phase, spatial and temporal profile modulation (electrical, optical, mechanical and thermal), including the employment of semiconductors and metamaterials [1] and, recently, one-atom-thick graphene [2–7]. Most of the proposed modulators, including graphene-based ones, are developed for free-space propagation configurations. A recently published paper [8] analyses the best performance limits of thin graphene-based reciprocal and non-reciprocal devices. However, high-speed THz/IR communication channels will unlikely be based on such architectures - atmospheric absorption peaks and small wavelengths (from sub-millimeter to tens of micrometers) imply strong free-space attenuation. It is therefore very natural to consider waveguide-based THz/IR modulators similar to those used in telecom photonics [9, 10].

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The electromagnetic character of graphene evolves from (1) highly resistive, to (2) low-loss inductive ($\text{Im}(\sigma) > 0$), then to (3) capacitive ($\text{Im}(\sigma) < 0$) and finally to (4) resistive again [17, 22, 23] (see Fig. 1(a)). At both microwave frequencies, regime (1), and optical frequencies, regime (4), $\text{Re}(\sigma)$ dominates over $\text{Im}(\sigma)$, however there is a fundamental difference between these states in terms of their response to graphene’s Fermi energy variations. In (1), electrochemical potential substantially influences $\text{Re}(\sigma)$, while in (4) the latter stays constant and equal to $\sigma_0 = e^2/4\hbar = 0.061$ mS. It is the THz/IR frequency range where the most dramatic changes take place - for every electrochemical potential value (Fermi energy level $E_F$), higher than a certain threshold value (around 26 meV), there is a frequency at which the imaginary part of graphene conductivity $\text{Im}(\sigma)$ becomes negative and decreases until reaching a minimal value at the frequency of Pauli blocking threshold ($\hbar \omega = 2E_F$) [22] (see Fig. 1(b)). At the same point, the real part of graphene conductivity $\text{Re}(\sigma)$ experience a step-like transition.

In this work, we study the effective electromagnetic properties of multilayer graphene in the vicinity of the above-mentioned transition region and develop a novel concept of a terahertz modulator consisting of a hollow waveguide filled with a graphene-dielectric metamaterial. We demonstrate an efficient, compact and ultrasensitive concept of a terahertz modulator consisting of a hollow waveguide filled with a graphene-dielectric metamaterial.

The electromagnetic properties of multilayer graphene-dielectric metamaterial. General consideration of modulation of terahertz radiation in a hollow waveguide filled with such medium is given in Section 3. Sections 4 and 5 present the design approaches yielding high ON-state transmission and high modulation depth, and extreme sensitivity towards graphene’s Fermi energy variation, respectively. Section 6 demonstrates the tunable passband filter performance of hollow waveguides filled with graphene/dielectric metamaterials. Finally, Section 7 concludes the article.

2. Multilayer graphene/dielectric metamaterial

We investigate the electromagnetic properties of a metamaterial formed by graphene sheets interlayed by dielectric spacers of thickness $d$ and dielectric permittivity $\varepsilon_M$ (Fig. 2). Similar metamaterial has recently been theoretically studied [24] and successfully fabricated using polymer spacers between graphene sheets with thicknesses of 20 nm, 100 nm, and 200 nm, respectively [25–27]. We suppose that initially all graphene layers are in the intrinsic state ($E_F = 0$ eV), and that each pair of graphene sheets is gated by applied voltage providing tunability of macroscopic electromagnetic properties of the structure. For example, it can be achieved by connecting even and odd

![Figure 1](image-url)
Figure 2  Tunable multilayer graphene metamaterial controlled by applied gate voltage. Graphene layers are separated with dielectric spacers with permittivity $\varepsilon_M$.

layers to positive and negative poles of the voltage source, respectively.

Assuming $d$ to be much smaller than the wavelength $\lambda$ of interest (for example, $d = 100 \text{ nm} \ll \lambda = 10 \mu\text{m}$), we can characterize the structure by an effective permittivity tensor. The electric field must be aligned with graphene layers in order to induce interaction with graphene’s surface conductivity. Thus, the out-of-plane component (perpendicular to graphene sheets) of the effective dielectric permittivity tensor equals to $\varepsilon_M$, and the in-plane permittivity components (with respect to graphene sheets) can be expressed as:

$$\varepsilon_{\text{eff}}(\varepsilon_M, \omega, d, E_f, \gamma) = \varepsilon_M + \frac{i\sigma(\omega, E_f, \gamma)}{\omega\varepsilon_0 d}, \quad (2)$$

where $\varepsilon_0$ is the permittivity of free space.

We can place such a metamaterial inside a hollow waveguide and, depending on the operating frequency band, build a waveguide-based modulator basing on various principles (Fig. 3(a)):

1. In the low frequency range, a graphene/dielectric metamaterial exhibits metallic behavior. Placed inside a waveguide with a mode polarised along graphene layers, such a medium acts as a shutter with tunable reflectivity.

2. An interesting epsilon-near-zero regime is possible around $\text{Re}(\varepsilon_{\text{eff}}) \approx 0$ - waves can then propagate through virtually any waveguide cross-section [28]. The zero-crossing of the real part of the effective dielectric permittivity of a graphene/dielectric metamaterial can be seen as a metal to dielectric transition.

3. A low-loss low-density dielectric regime with $0 < \text{Re}(\varepsilon_{\text{eff}}) < \varepsilon_M$ can be observed at frequencies slightly below $\omega = 2E_F/\hbar$. In this regime, modes of hollow waveguides filled with this graphene/dielectric metamaterial can propagate with very low attenuation.

4. A low-loss high-density dielectric regime with $\varepsilon_M > \text{Re}(\varepsilon_{\text{eff}})$ can be observed at frequencies around the Pauli blocking threshold $\omega = 2E_F/\hbar$. Since every variation of graphene’s electrochemical potential will change the effective refractive index of the waveguide core, it will dramatically influence the transmission of small waveguides (slightly above the cut-off). It is then possible to arrange controllable switching between below-cut-off and propagating regimes for their modes.

5. At higher frequencies $\omega > 2E_F/\hbar$, a graphene/dielectric metamaterial undergoes an abrupt transition to lossy dielectric material. We can benefit from the dependence of this sharp step-like transition on the Fermi energy, and control the waveguide mode attenuation due to absorption in the waveguide filling material.

The exact spectral locations of all the abovementioned changes in graphene’s conductivity depend on the concentration of its charge carriers, which is directly connected to its Fermi energy level (Fig. 3(b)). The latter is governed by the gate voltage. In this work, we use the kink-like behavior of losses and the significant refractive index change in the vicinity of $\omega = 2E_F/\hbar$, as well as graphene’s metal to dielectric transition to influence the propagation of waves in a waveguide filled with a graphene-dielectric metamaterial. This approach allows us to achieve electrically controllable waveguide-based modulation at the THz frequencies.
3. Hollow waveguide filled with graphene/dielectric metamaterial

We consider a hollow rectangular waveguide filled with multilayer graphene (Fig. 4). The level of ohmic losses in single-mode micro-sized metallic waveguides at 30 THz is around $0.015 - 0.016 \text{ dB/}\mu\text{m}$ for cores with linear sizes of several micrometres [29]. To ensure low losses, hollow THz waveguides typically have a dielectric lining [12,13]. In this paper, we disregard ohmic losses and consider ideal (made of perfect electric conductor) hollow waveguides in order to focus on the effects brought by the graphene multilayer core.

We wish our modulating waveguide section to transmit a single fundamental mode in the ON-state (Fig. 4(b)) [30]. We also wish this mode to be suppressed in the OFF-state due to either metallic behavior of the composite ("mode killer"), large absorption or waveguide cut-off conditions. As discussed in the previous Section, transitions between the electromagnetic regimes of graphene, and thus the modulation, can be achieved by changing the applied gate voltage. Since we consider initially intrinsic graphene layers assuming certain freedom of choice regarding the dielectric material interlaying graphene sheets, we can engineer the graphene/dielectric metamaterial in such a way that its resulting effective refractive index in the ON-state coincides with that of a transparent material filling the input and output waveguides. This would ensure perfect matching and minimize insertion loss of the modulating system. The use of hollow input and output metallic waveguides with filling refractive index $n_{\text{on}} = 1$ is possible, however very low-index material between graphene layers would be required. A more down-to-earth solution consists in using well-known IR materials, such as CsBr ($n = 1.663$), CsI ($n = 1.739$) and NaCl ($n = 1.495$) [31], both for the graphene/dielectric metamaterial spacer and the filling for the input and output waveguides. Apart from their relatively low price, all these substances demonstrate excellent IR transmission and allow the fabrication of thin films with thicknesses of several nanometers [32,33]. Recently reported direct growth of graphene on Ge films [34] can be a potential option for multilayer graphene metamaterials, especially taking into account the transparency and low losses of Ge in the frequency range of interest [31]. Nevertheless, direct fabrication of a Ge-graphene composite is challenging and the use of this optically dense material would imply decreasing the distances between graphene layers to less than ten nanometers and substantially shrinking the size of the embedding, input and output waveguides.

4. Waveguide modulator with high modulation depth

Dielectric properties of the metamaterial described in Section 2 would obviously depend on the distance between the graphene sheets. In turn, the resulting refractive index at the desired ON-state frequency determines the dimensions of the waveguide $a \times b$ (see Fig. 4). To ensure the single-mode regime, the waveguide dimensions should fall between the TE$_{10}$ and TE$_{20}$ cut-off conditions (the first mode propagates, while the second still does not). Aiming at achieving the best possible transmission in the modulator’s ON-state, one should look for the Fermi energy level corresponding to the minimum of the mode amplitude attenuation coefficient $\alpha_s$, $E_{f \text{min}}(\alpha)$. Figure 5(a) shows the real parts of the refractive indices of the graphene/CsBr multilayer metamaterials, plotted against the distances between graphene sheets for different waveguide widths $a$. Each curve represents the values of $n_{\text{eff}}(d) \mid E_{f} = E_{f \text{min}}(\alpha)$ at Fermi energy values $E_f$ corresponding to the minima of the fundamental mode amplitude attenuation constant (red curve in Fig. 5(b)). Since we wish to stay in the single-mode regime, the first- and second-order mode cut-off conditions are taken into account - the solid lines end at cut-off conditions (the dashed curves are to guide the eye). Having defined the desired ON-state refractive index of the metamaterial, one can pick the appropriate waveguide width and find the corresponding distance between graphene sheets (marked by the black circle). For our example, we set the width of the waveguide equal to 5 $\mu$m, and the thicknesses of the dielectric spacers ensuring perfect matching to the NaCl input and output waveguides equal to 51 nm. The height of the waveguide should ensure the absence of propagating cross-polarised waveguide modes, for example, $b = 2.5$ $\mu$m. The Fermi energy corresponding to the ON-state of this device is $E_{f(\text{on})} = 111$ meV. Figure 5(b) shows the analytically calculated inverse amplitude attenuation coefficient of the TE$_{10}$ mode of a hollow rectangular waveguide filled with multilayer graphene (a material with complex $n_{\text{eff}}$). Additional curves on the graph indicate the location of the above mentioned mode cut-off conditions as well as the local minimum of $\alpha$.

Once the desired transmission is defined, the length of the waveguide modulator section is determined as:

$$L = -\frac{1}{2\alpha_{\text{on}}} \ln T_{\text{on}}$$

(3)
Real part of the refractive index of the graphene/CsBr metamaterial vs. distance between graphene sheets at temperature $T = 300$ K. Each curve corresponds to the minimal TE$_{10}$ attenuation condition, and is plotted for the indicated waveguide width and continued by a dashed curve below the cut-off conditions. Inverse amplitude attenuation coefficient, $\alpha^{-1} (\mu m^{-1})$, of the TE$_{10}$ mode of a graphene/CsBr-filled waveguide ($d = 51$ nm) as a function of the waveguide width $a$ and graphene’s Fermi energy $E_F$. The red curve corresponds to the local minima of $\alpha$. Dark grey and light grey curves denote the cut-off conditions of the TE$_{10}$ and TE$_{20}$ modes, respectively.

For example, a 95% power transmission in a 5 $\mu$m-wide waveguide filled with the graphene/CsBr metamaterial can be achieved at $L = 13.34 \mu m$ ($\approx 1.3\lambda$). Figure 6(a) shows how the modulation depth (calculated as the absolute value of the ON- and OFF-state transmission coefficients ratio) of this modulator waveguide section depends on the change of the graphene’s Fermi energy $\Delta E_F$. A high modulation depth, above 25 dB, is observed when graphene’s electrochemical potential shifts by a value as small as $\sim 50$ meV. Further decrease in the Fermi energy yields modulation depth values of 36 dB and $> 38.5$ dB at $\Delta E_F = -60$ meV and $\Delta E_F = -90$ meV, respectively. The graphene’s conductivity model used in this paper ($E_F > k_B T$ assumption) is valid for simulating the modulator performance at Fermi energies above $E_F \approx 26$ meV [35]. Of course, shorter modulator sections would give even better transmission at the cost of modulation depth degradation. Looking back at Fig. 5(b), one may notice that not only negative Fermi energy shifts lead to waveguide mode attenuation. Increasing the Fermi energy also allows for modulation, however, at larger values of $\Delta E_F$. As seen from the corresponding changes in the effective refractive index of the simulated graphene metamaterial plotted in Fig. 6(b), a negative $\Delta E_F \approx -50$ eV corresponds to an abrupt increase of attenuation. At the same time, positive $\Delta E_F \approx 100$ eV makes the metamaterial in the waveguide modulator section metallic impeding the propagation of any waves through the device.

The graphene/CsBr waveguide modulator connected to NaCl-filled input and output waveguides was simulated using CST [36]. Its numerically obtained transmission coefficients and electric field profiles in the ON- and OFF-states are shown in Figs. 7 and 8, respectively. This example demonstrates the excellent performance of the proposed terahertz modulator: a 70 meV shift of the graphene’s Fermi energy level leads to the complete and immediate switch between transmission and attenuation regimes. Moreover, the modulation is broadband.

Figure 5 (a) Real part of the refractive index of the graphene/CsBr metamaterial vs. distance between graphene sheets at temperature $T = 300$ K. Each curve corresponds to the minimal TE$_{10}$ attenuation condition, and is plotted for the indicated waveguide width and continued by a dashed curve below the cut-off conditions. (b) Inverse amplitude attenuation coefficient, $\alpha^{-1} (\mu m^{-1})$, of the TE$_{10}$ mode of a graphene/CsBr-filled waveguide ($d = 51$ nm) as a function of the waveguide width $a$ and graphene’s Fermi energy $E_F$. The red curve corresponds to the local minima of $\alpha$. Dark grey and light grey curves denote the cut-off conditions of the TE$_{10}$ and TE$_{20}$ modes, respectively.

Figure 6 (a) Modulation depth vs. graphene Fermi energy change $\Delta E_F$ for graphene/CsBr metamaterial at $E_F^{(ON)} = 111$ meV, $a = 5 \mu m$ and $L = 13.34 \mu m$. The transmittance is set as $T_{\text{ON}} = 95\%$. (b) Effective refractive index of the simulated graphene/CsBr metamaterial. A negative shift of the Fermi energy level ($\approx -50$ meV) leads to attenuation via dielectric losses, while a slightly bigger positive shift ($\approx 100$ meV) converts the modulating section into a metallic block.
5. Waveguide modulator with extreme sensitivity

For certain applications achieving extremely high sensitivity can be prioritised above minimal mode attenuation. We define a Figure-of-Merit (FoM) characterizing the tradeoff between the sensitivity and losses as follows:

\[ FoM = \left| \frac{1}{\alpha} \frac{\partial \alpha}{\partial E_f} \right| \]

(4)

Let us assume that the dielectric layers between the graphene sheets in out metamaterial are made of NaCl \((n = 1.495)\). Following the same steps as those described in the previous Section, it is possible to define the distance between graphene sheets providing a pre-defined effective refractive index in the ON-state. It is also important to re-adjust the width of the waveguide in order to meet the cut-off conditions. In our sample design, we have chosen CsI \((n = 1.739)\) as an input/output waveguide filling material. For a 5 \(\mu\)m-wide waveguide, the perfect matching with a CsI filled input waveguide occurs at \(d = 44.5\)nm.

In the following Sections, we will consider low temperatures \((10\) K\) to ensure that thermal fluctuations do not affect the performance of our devices as we reach the switching energies of several meV.

It can be seen from Fig. 9(a) that a slight variation of the gate voltage can significantly change the dielectric properties of the waveguide core leading to strong attenuation of the fundamental mode. The modulation depth plotted against Fermi energy change is shown in Figs. 9(b) and 9(c).

At \(E_{f,\text{on}} \approx 62\) meV, where a local maximum of the FoM of graphene/CsBr metamaterial is located, the transmission coefficient of a 10 \(\mu\)m-long \((1\lambda)\) modulator section in the ON-state is \(-11.91\) dB. A 1 meV increase of graphene’s Fermi energy leads to \(+6.82\) dB improvement of the modulator transmission. A negative shift of \(-1\) meV of graphene’s Fermi energy makes the modulator transmission \(-12.25\) dB worse. Similarly, positive and negative shifts of 2 meV in the Fermi energy level lead to a \(+8.76\) dB and \(-16.74\) dB shifts in the transmission coefficient, respectively. Another local maximum of the FoM of the considered graphene/NaCl metamaterial waveguide is located at \(E_{f,\text{on}} \approx 172\) meV. The transmission coefficient of a 10 \(\mu\)m-long \((1\lambda)\) modulator section in this ON-state is \(-8.88\) dB. Comparing Figs. 9(b) and 9(c), one can conclude that the sensitivity is slightly lower than in the previously described case. Indeed, positive 1 meV and 2 meV shifts in the Fermi energy level lead to \(+9.14\) dB and \(+16.08\) dB modulation depth values, respectively. The advantage of this local minimum is the possibility to dramatically increase the modulation depth of the device: for instance, a 50 meV increase of graphene’s Fermi energy would lead to an extraordinary value of \(+140\) dB modulation depth. It is important to remember, however, that in this case, due to metallic behavior of the core, the energy would bounce back to the source rather than be absorbed by the modulating section.

Such extreme sensitivity makes graphene a very promising platform for designing energy-efficient high-speed and compact waveguide-based modulators and other functional devices in the THz/IR frequency range.

6. Tunable waveguide-based passband filter

As shown in Section 2, for any (high enough) value of the graphene’s Fermi energy, there is a region of frequencies where the effective refractive index of the metamaterial \(n_{\text{eff}}\) exceeds that of the spacer between the graphene sheets \(n_{M}\). Its maximal value at the Pauli blocking treash-
old falls on the middle of the attenuation coefficient slope (Fig. 10(a)). At these frequencies, even if the width of the modulating waveguide is smaller than \( \lambda^2 \) (TE\(_{10}\) mode cut-off condition), its fundamental mode can be squeezed into the waveguide cross-section. We propose to use this phenomenon to create a tunable graphene-based passband filter. The lower cutoff frequency of the resulting passband device is defined by the cut-off condition for the fundamental mode at \( n_{eff} = n_M \). At higher frequencies, it is attenuated due to quickly increasing losses in graphene - this forms the upper limit of the passband. Changes in the graphene’s Fermi energy level simultaneously shift these frequencies converting the resulting device into a tunable passband filter. Once the desired central frequency of the tunable device is defined, the parameters of the metamaterial, the width of the waveguide and the ON-state graphene’s Fermi energy should be chosen as explained in Section 4. Fig. 10(b) shows the numerically calculated transmission coefficients of the graphene/NaCl metamaterial described in Section 4 connected to the CsI-filled input and output waveguides. It demonstrates the possibility to tune the passband of this waveguide filter by changing the applied gate voltage. Central frequency shift of order of 5% is observed at \( \Delta E_f = 4 \text{ meV} \) together with a bandwidth decrease.

7. Conclusions

The interplay between interband and intraband transitions in graphene allows converting a multilayer graphene/dielectric structure into a transparent and/or electromagnetically dense artificial medium in a narrow THz/IR frequency range. The gate voltage can be used to electrically control the concentration of carriers in the graphene sheets and, thus, efficiently change the dispersion of the whole structure. Placed inside a hollow waveguide, a multilayer graphene/dielectric metamaterial provides high-speed modulation of radiation and offers novel concepts for terahertz modulators and tunable bandpass filters. We show the possibility to design waveguide-based terahertz modulators with high ON-state transmission and competitive energetic efficiency: with a 50 meV shift of graphene’s Fermi energy, it is possible to switch between transmission and attenuation regimes. We also demonstrate the extreme sensitivity of graphene-based waveguide modulators - extraordinary...
values of 12 dB/meV can be achieved. In the same configuration, one can also design a passband waveguide-based filter able to shift its central frequency by 1.24% per every meV of the graphene’s Fermi energy variation. In this work, we considered only a single-mode waveguide. Much more possibilities appear when using a multimode waveguide, so the tunable graphene dielectric composite, especially not covering the whole waveguide cross-section, can act as a tunable attenuator, or mode and/or polarisation selector. We wish to emphasise the choice of a hollow metallic waveguide as the core element of the modulator. Being confined with the impermeable metallic walls, the wave in the OFF-state can either be absorbed or reflected back, but not scattered to the surrounding space, contrary to what occurs in dielectric waveguides. The absence of scattered radiation enables dense integration of such THz waveguides and modulators without influencing their neighbouring elements. We believe that graphene-dielectric multilayer composites will constitute a useful functional element for the THz-IR waveguide-integrated devices.

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References