Discussion of temperature-dependent epsilon-near-zero effect in graphene

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Abstract

In the present paper, we discuss the temperature-dependent epsilon-near-zero (ENZ) effect in graphene arising in the framework of its isotropic model. The effect was theoretically investigated in detail using a simplified model design of the slot line containing a graphene layer in which all other effects are eliminated allowing us to focus solely on the ENZ effect. With the reduction of graphene effective temperature, the ENZ effect in the near-IR wavelength range was found to become pronounced even for structures and metasurfaces for which it has been considered neglectable and has not been previously observed at room temperatures. This temperature-dependent behaviour was interpreted analytically within the approximation in which the real part of the graphene dielectric constant is considered vanishingly small compared to the imaginary part (this condition is always satisfied at the ENZ point in graphene).

1. Introduction

Graphene-supported devices and metadevices have been intensively investigated to be used in the fields ranging from electronic–photonic integrated circuits and all-optical switches/modulators to biosensors [1–9]. In addition, the epsilon-near-zero (ENZ) effect arising in graphene being considered as a 3D isotropic material [10] has been also considered in transverse magnetic (TM)-modes-supporting devices to further increase their performance [11–16]. Besides, the optical properties of graphene were also theoretically studied considering it as an isotropic material [17, 18]. At the same time, despite controversial results and still ongoing dispute if the ENZ effect can exist in graphene in reality [10, 19–22], the controversial nature of the isotropic graphene model has never been considered as an issue for devices designed to be used without TM-modes as fundamental/guided modes (i.e., devices with guided modes which electric field components lie in the plane of graphene layer)—this is due to the fact that under this condition ENZ effect in graphene is considered neglectable and has been never observed in such kind of devices in the near-IR wavelength range at room temperatures [3, 23]. In other words, the isotropic graphene model has been considered applicable without any concerns for such kind of devices. However, willing to reveal the real nature of the temperature-dependent modulation effect shown in [23], in the present work we highlight that with the reduction of graphene effective temperature, the ENZ effect in the near-IR wavelength range becomes essential even for such kind of structures and can greatly affect their performance. This temperature-dependent behaviour was interpreted analytically within the approximation when the real part of the graphene dielectric constant is considered vanishingly small compared to the imaginary part (this condition is always satisfied at the ENZ point in graphene).
2. Details of the theoretical analysis

2.1. Model of the considered problem

The original design of the graphene-based modulator considered in [3, 23] is shown in figure 1. A plane wave with the electric field polarization along x- or y-axis (i.e., lying in the plane of the graphene layer) propagating in the negative direction along z-axis excites the structure. In [23] it was shown that under specific values of the graphene effective temperature $T$ and chemical potential $\mu_c$, the propagating wave acquires an increased absorption which allowed to increase the modulation depth of the device up to three times. However, the real nature of the modulation was not revealed, and (in accordance with the obtained results) the effect was attributed to an additional resonance excitation in the graphene layer (e.g., a plasmonic one). The observed effect was almost impossible to relate at that moment to the ENZ effect in graphene due to the geometrical and electromagnetic configuration of the problem.

Using the original design (shown in figure 1), it is extremely difficult to interpret results obtained in [23] due to the fact that it contains two slot lines (orthogonal to each other) that form a cross-shaped structure, and this cross-shaped structure is excited by the plane wave simultaneously all over the structure’s surface. At the same time, due to the symmetry of the considered geometry, one of the slot lines (which is extended along the plane wave polarization) cannot qualitatively affect the observed results. Therefore, in the present work, we replaced the original design with a model one (this model with notations and dimensions is shown in figure 2). The model design is a single slot line rotated by $\pi/2$ (in respect to the slot line of the original design) in order to be extended along the excitation mode propagation. A short section (1000 nm long) of the slot line with strips made of the perfect electric conductor was added at the beginning of the line to be able to launch the fundamental quasi transverse electro-magnetic (TEM) mode at the Ag-strips line beginning (see figure 3). This model design allows one to excite the quasi-TEM mode of the slot line from one side and analyse its propagation along the line while changing the graphene physical parameters. Importantly that all other electromagnetic configuration features (such as excitation wave polarization relative to the graphene layer) remain intact in the model design.

Numerical simulations were performed in the frequency domain (finite element method). The following parameters were used for the design model: the width $w$ of the slot line is 90 nm; thickness of the Ag layer is 100 nm; thickness of the SiO$_2$ buffer dielectric layer is 10 nm; thickness of the graphene layer $\Delta$ is 0.34 nm. Worth to note that all slot line parameters (such as width $w = 90$ nm and thickness of the Ag layer of 100 nm) were kept the same as for the original design. An adaptive mesh convergence analysis was carried out before the main investigation (see figure S1 (https://stacks.iop.org/NJP/24/083016/mmedia) in supporting information).

2.2. Parameters of the graphene layer

Graphene, a monolayer of carbon atoms, is considered to have a finite thickness $\Delta$ of 0.34 nm. Its effective dielectric constant $\varepsilon_g$ can be represented by a diagonal tensor with in-plane components $\varepsilon_{xx}$ and $\varepsilon_{yy}$ and a component $\varepsilon_{zz}$ (which is normal to the graphene surface in our configuration). In-plane components $\varepsilon_{xx}$ and $\varepsilon_{yy}$ can be calculated as [10]

$$
\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{||\infty} + \frac{i \sigma ||}{\omega \varepsilon_0 \Delta},
$$

(1)
Figure 2. 3D (a) front and (b) back views and (c) 2D front-view schematic of the model design with notations and dimensions.

Figure 3. Magnitudes of the (a) absolute value, (b) $x$-component, and (c) $z$-component of the electric field of the fundamental quasi-TEM-mode. The scale bar is 100 nm.

where $\varepsilon_0$ and $\varepsilon_{\parallel\infty}$ are vacuum and background dialectic constants, respectively, $\omega$ is radian frequency, and $\sigma_{\parallel}$ is graphene in-plane conductivity. In the similar way, surface-normal component $\varepsilon_{zz}$ can be calculated via the graphene surface-normal conductivity $\sigma_{\perp}$ as

$$
\varepsilon_{zz} = \varepsilon_{\perp\infty} + i \frac{\sigma_{\perp}}{\omega \varepsilon_0 \Delta},
$$

(2)

where $\varepsilon_{\perp\infty}$ is background dialectic constant. In many cases, it can be assumed that $\varepsilon_{\parallel\infty} = \varepsilon_{\perp\infty}$. Besides, in the framework of graphene isotropic model, $\sigma_{\parallel} = \sigma_{\perp}$ and, therefore, from equations (1) and (2): $\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz}$. In this case, given the graphene (isotropic) surface conductivity $\sigma_{g}$ [24, 25], its effective dielectric constant $\varepsilon_{g}$ can be deduced as

$$
\varepsilon_{g} = 1 + i \frac{\sigma_{g}}{\omega \varepsilon_0 \Delta}.
$$

(3)

Carrier density $n$ in graphene can be tuned by varying the chemical potential $\mu_c$ which, in turn, can be actively tuned by varying the applied voltage $V_g$ [3, 23, 26]. Therefore, real and imaginary parts of the graphene dielectric constant $\varepsilon_{g}$ can be tuned by changing its chemical potential $\mu_c$ (see figure 4). As it is seen from figure 4, the permittivity of graphene reaches the ENZ point ($\varepsilon_{g} = -0.019 + i0.411$) at $\mu_c = 0.5$ eV and $f = 193$ THz ($\lambda = 1.553$ $\mu$m), however this effect was not observed in ‘non-TM-mode’ devices at room temperatures [3, 23] (this issue has been described above). Electron relaxation time in graphene, $\tau$, was set to 0.1 ps for all values of the temperature $T$. 

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3. Results and discussion

Figures 5(a) and (b) show distribution of the $x$-component of the electric field along the center of the slot line ($x = 0, z = 0$—see figures 2 and 3) for the cases of $T = 293.15 \text{ K}, f = 193.000 \text{ THz}$ and $T = 135.25 \text{ K}, f = 191.573 \text{ THz}$, respectively. Frequency $f$ of 191.573 THz for $T = 135.25 \text{ K}$ was chosen as it corresponds to the point of anomalous absorption observed in [23] and it was found that permittivity of graphene reaches the ENZ point ($\varepsilon_g = 0.015 + i0.115$) at $\mu_c = 0.489 \text{ eV}$ for these values of $f$ and $T$ (see figure S2). Electric field distribution shown in figures 5(a) and (b) are typical standing waves formed by forward and backward (reflected from the line terminal) waves. In addition, in figures 5(a) and (b) dashed lines connecting third and fifth antinodes and second and fourth nodes (relatively to the line beginning) are shown. Due to the fact that conditions at the slot line terminal are the same for all values of $\mu_c$ (and, therefore, return loss values are the same in all cases), the slope of these lines can be used to characterize the linear losses in the slot line for different values of the graphene chemical potential $\mu_c$. For more clearance, insets for figure 5 are presented in figure S4. From figure S4 it is clear that at ENZ points ($\mu_c = 0.500$ and 0.489 eV for figures S4(a) and (b), respectively) linear loss increases sharply, which leads to an increased absorption of the quasi-TEM mode of the slot line. It is also clear from figure 5 that at $T = 135.25 \text{ K}$ linear loss increases much greater than that at $T = 293.15 \text{ K}$.

Increased linear loss observed in figure S4 cannot be attributed to a plasmonic resonance excitation in graphene because under such conditions real part of the graphene dielectric constant (see figures 4 and S2)...
do not satisfy the plasmonic dispersion relation. However, due to the fact that this increased linear loss occurs at ENZ points of graphene, it can be related to the ENZ effect in graphene despite the fact that $z$-component of the quasi-TEM mode electric field (which is orthogonal to the graphene layer) is negligible all over the slot line cross-section except for the edges of the metallic strips (see figure 3(c)). To test this assumption, we examined electric field distributions in the plane orthogonal to the quasi-TEM mode propagation and coming across fourth of the considered in figure 5 antinodes. $E_x$- and $E_z$-field distributions for different frequencies in plane of $y = 2287$ nm in the case of $T = 135.25$ K, $\mu_c = 0.489$ eV are depicted in figures 6(a) and (b), respectively. In figure 6, the very left pictures are overall views at $f = 180$ THz and right pictures are magnified views of the corner marked by white circle in the left pictures for different frequencies.

From figure 6(a) it is clear that magnitude of the $E_x$-component of the quasi-TEM mode is slightly lowered at $f = 191.573$ THz. At the same time, at $f = 191.573$ THz, $E_z$-component starts to concentrate almost completely in the graphene layer (which is a property of the ENZ effect). This effect can be understood from the following consideration: the field amplitude in the one optical medium ($\varepsilon'_a$) relatively to another one ($\varepsilon'_b$) can be increased (close to their interface or in the volume in the case of a thin layer) if the ratio of $|\varepsilon'_a/\varepsilon'_b|$ is large. This is attributable to the discontinuity of the normal components of the electric field at the interface: $D_{na} = D_{nb} \Rightarrow E_{na}\varepsilon'_a = E_{nb}\varepsilon'_b \Rightarrow E_{nb} = |\varepsilon'_a/\varepsilon'_b|E_{na}$. If the medium $b$ is lossy ($\varepsilon''_b > 0$), then the field undergoes propagation loss which is proportional to $E_{nb}\varepsilon''_b$ (for the exact expression, see equation (4)) below.

To make results presented in figure 6 more clear, distributions of the electric field $E_z$-component along the white horizontal dashed line (see left picture in figure 6(b)) for different frequencies are presented in figures S5(a) (figure 7(a) shows the inset of figure S5(a)). On the contrary, there is no ENZ effect at $T = 135.25$ K and $\mu_c = 0.100$ eV (see figures S5(b) and 7(b)).

It is important to note here that the same behaviour shown in figures 6 and 7 in the case of $T = 135.25$ K, $\mu_c = 0.489$ eV was observed in the case of $T = 293.15$ K, $\mu_c = 0.500$ eV. However, the question is arising here—why ohmic loss is so drastically different in both cases (see figure 8 where ohmic
losses in graphene for both cases are shown) which leads to the observed fact that ENZ effect almost does not appear at room temperatures and was not observed for the considered modulator geometries [3, 23] while it exists in principle under such conditions. Especially, taking into account that in the case of $T = 293.15 \, \text{K}, \mu_c = 0.500 \, \text{eV}$ imaginary part of the graphene $\varepsilon_g$ is about 4 times higher than that for $T = 135.25 \, \text{K}, \mu_c = 0.489 \, \text{eV}$ (see figure S3 and table 1).

While it appears senseless under the ‘normal’ operation, at the ENZ effect a condition of $|\varepsilon'| \ll \varepsilon''$ is occurred and, when this condition is satisfied, decreasing of the imaginary part can lead to the ohmic loss increasing. To understand this, consider a capacitor filled with vacuum and having a thin lossy layer inside it, to which a varied voltage is applied. Ohmic losses in the lossy layer can be calculated as:

$$P = \text{Re} \left\{ \frac{1}{2} \int_{V_l} E \vec{j}^* \, \text{d}V \right\} = \frac{\omega \varepsilon_0}{2} \int_{V_l} \varepsilon'' E^* E \, \text{d}V, \quad (4)$$

where $\vec{E}$ is the electric field in the layer, $\vec{j}^*$ is the complex conjugate current density and the integration is carried out over the entire volume of the layer $V_l$. Consider the electric field in the layer: in approximation

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**Table 1.** Real ($\varepsilon'$) and imaginary ($\varepsilon''$) parts of the graphene $\varepsilon_g$

|           | $T = 293.15 \, \text{K}, \mu_c = 0.500 \, \text{eV}$ | $T = 135.25 \, \text{K}, \mu_c = 0.489 \, \text{eV}$ |
|-----------|------------------------------------------------------|------------------------------------------------------|
| $\varepsilon'$ | -0.019                                               | 0.015                                                 |
| $\varepsilon''$ | 0.411                                                | 0.115                                                 |
of a thin layer, electric fields above and below the layer are the same: \( E_0 = V_g/h \), where \( V_g \) is the applied voltage and \( h \) is a distance between the capacitor plates. For the electric field component orthogonal to the layer at the interface between air and the layer one can write therefore:

\[
D_{\perp 0} = D_{\perp d} = E_0 = E \varepsilon_i,
\]

where \( \varepsilon_i \) is a complex dielectric constant of the layer. Therefore, \( \mathbf{E} = \mathbf{E}_0/\varepsilon \) and substituting this into the equation (4), one obtains:

\[
P = \text{Re} \left( \frac{1}{2} \int_{V_l} \mathbf{E} \cdot \mathbf{j} \, dV \right) = \frac{\omega \varepsilon_0}{2} \int_{V_l} \frac{E_0 E_0^*}{\varepsilon''} \, dV.
\]

In the approximation of \( |\varepsilon'| \ll \varepsilon'' \) (which always takes place at the ENZ point), one can rewrite equation (6) as follows:

\[
P = \text{Re} \left( \frac{1}{2} \int_{V_l} \mathbf{E} \cdot \mathbf{j} \, dV \right) = \frac{\omega \varepsilon_0}{2} \int_{V_l} \frac{E_0 E_0^*}{\varepsilon''} \, dV.
\]

From equation (7) is it thus clear that decreasing of the imaginary part \( \varepsilon'' \) of the lossy layer can lead to the ohmic loss increasing inside it.

This analysis can account for the observed ohmic loss increasing (see figure 8) at the decreased graphene effective temperature \( T \)—because at the decreased \( T \) real and imaginary part curves come closer to each other at the ENZ point (see figure S3) which, in turn, leads to a significant imaginary part decreasing (see table 1) at that point and, therefore, to the ohmic loss increasing (according to equation (7)).

4. Conclusion

ENZ effect may arise in graphene if its effective dielectric constant is treated as an isotropic one, i.e., \( \varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz} \) (called the graphene isotropic model). Despite still ongoing dispute if it is possible for the ENZ effect to exist in graphene in reality [10, 19–22], the controversial nature of the graphene isotropic model has never been considered as an issue for devices designed to be used without TM-modes as fundamental/guided modes. Therefore, the graphene isotropic model has been considered as applicable without any concerns for such kind of devices. In the present paper, we however showed that the ENZ effect in the near-IR wavelength range can arise in graphene even in these structures with reducing the graphene effective temperature. The observed temperature-dependent behaviour was interpreted analytically within the approximation when the real part of the graphene dielectric constant is considered vanishingly small in comparison with the imaginary part (this condition is always satisfied at the ENZ point in graphene). The obtained results show the conditions when ENZ in graphene is more pronounced and, therefore, they may be potentially helpful in the construction of an experiment designed to finally prove or disregard the applicability of the isotropic model of graphene. This study can thus significantly contribute to the field of investigation of the fundamental properties of graphene.

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Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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References

[1] Zheludev N I and Kivshar Y S 2012 From metamaterials to metadevices Nat. Mater. 11 917–24
[2] Liu M, Yin X, Ulin-Avila E, Geng B, Zentgraf T, Ju L, Wang F and Zhang X 2011 A graphene-based broadband optical modulator Nature 474 64–7
[3] He X, Zhao Z-Y and Shi W 2015 Graphene-supported tunable near-IR metamaterials Opt. Lett. 40 178–81
[4] Low T and Avouris P 2014 Graphene plasmonics for terahertz to mid-infrared applications ACS Nano 8 1086–101
[5] Aznakayeva D E, Rodriguez F J, Marshall O P and Grigorenko A N 2017 Graphene light modulators working at near-infrared wavelengths Opt. Express 25 10255–60
[6] Ono M, Hata M, Tsunekawa M, Nozaki K, Sumikura H, Chiba H and Notomi M 2020 Ultrafast and energy-efficient all-optical switching with graphene-loaded deep-subwavelength plasmonic waveguides Nat. Photon. 14 37–43
[7] Vakil A and Engheta N 2011 Transformation optics using graphene Science 332 1291–4
[8] Aspermair P et al 2020 Dual monitoring of surface reactions in real time by combined surface-plasmon resonance and field-effect transistor interrogation J. Am. Chem. Soc. 142 11709–16
[9] Xiao S, Wang T, Liu T, Zhou C, Jiang X and Zhang J 2020 Active metamaterials and metadevices: a review J. Phys. D: Appl. Phys. 53 503002
[10] Kwon M-S 2014 Discussion of the epsilon-near-zero effect of graphene in a horizontal slot waveguide IEEE Photon. J. 6 6100309
[11] Shin J-S and Kim J T 2015 Broadband silicon optical modulator using a graphene-integrated hybrid plasmonic waveguide Nanotechnology 26 365201
[12] Lee S, Tran T Q, Kim M, Heo H, Heo J and Kim S 2015 Angle- and position-insensitive electrically tunable absorption in graphene by epsilon-near-zero effect Opt. Express 23 33350–8
[13] Phatak A, Cheng Z, Qin C and Goda K 2016 Design of electro-optic modulators based on graphene-on-silicon slot waveguides Opt. Lett. 41 2501–4
[14] Lu H, Gan X, Mao D and Zhao J 2017 Graphene-supported manipulation of surface plasmon polaritons in metallic nanowaveguides Photon. Res. 5 162–7
[15] Feng Y, Hu Z-D, Balmakou A, Khakhomov S, Semchenko I, Wang J, Liu D and Sang T 2020 Perfect narrowband absorber based on patterned graphene-silica multilayer hyperbolic metamaterials Plasmonics 15 1869–74
[16] Caligiuri V, Pinelli A, Miscuglio M, Patra A, Maccaferri N, Caputo R and De Luca A 2020 Near- and mid-infrared graphene-based photonic architectures for ultrafast and low-power electro-optical switching and ultra-high resolution imaging ACS Appl. Nano Mater. 3 12218–30
[17] Falkovsky L A and Pershoguba S S 2007 Optical far-infrared properties of a graphene monolayer and multilayer Phys. Rev. B 76 155410
[18] Hanson G W 2008 Dyadic Green’s functions and guided surface waves for a surface conductivity model of graphene J. Appl. Phys. 103 064302
[19] Santos E J G and Kaxiras E 2013 Electric-field dependence of the effective dielectric constant in graphene Nano Lett. 13 898–902
[20] Hao R, Jin J, Wei X, Jin X, Zhang X and Li E 2014 Recent developments in graphene-based optical modulators Front. Optoelectron. 7 277–92
[21] Fang J, Vandenberge W G and Fischetti M V 2016 Microscopic dielectric permittivities of graphene nanoribbons and graphene Phys. Rev. B 94 045318
[22] de Oliveira R E P and de Matos C J S 2015 Graphene based waveguide polarizers: in-depth physical analysis and relevant parameters Sci. Rep. 5 16949
[23] Morozov Y M, Lapchuk A S, Protsak I S, Kryuchyn A A and Nevirkovets I P 2022 Temperature-dependent effect of modulation in graphene-supported metamaterials New J. Phys. 24 043006
[24] Gusynin V P, Sharapov S G and Carbotte J P 2006 Magneto-optical conductivity in graphene J. Phys.: Condens. Matter. 19 026222
[25] Luo X, Qiu T, Lu W and Ni Z 2013 Plasmons in graphene: recent progress and applications Mater. Sci. Eng. R 74 351–76
[26] Hanson G W 2008 Dyadic Green’s functions for an anisotropic, non-local model of biased graphene IEEE Trans. Antennas Propagat. 56 747–57