Contents lists available at ScienceDirect

## Materials Letters

journal homepage: www.elsevier.com/locate/matlet

# Modeling of 2D graphene material for plasmonic hybrid waveguide with enhanced near-infrared modulation

Jinfeng Zhu<sup>a,\*</sup>, Junjun Cheng<sup>a</sup>, Lirong Zhang<sup>a</sup>, Qing Huo Liu<sup>b,\*</sup>

<sup>a</sup> Department of Electronic Science, Xiamen University, Xiamen 361005, China

<sup>b</sup> Department of Electrical and Computer Engineering, Duke University, Durham, NC 27708, USA

#### ARTICLE INFO

*Keywords:* Simulation and modeling Carbon materials Optical materials and properties

### ABSTRACT

Modulating near-infrared signals is critical for high density optical interconnects. In order to achieve enhanced modulation effects, we design a near-infrared modulator in combination with a gold nanostripe waveguide and graphene. Conventional assumption of isotropic permittivities for graphene leads to exaggeration of light absorption at the so-called "epsilon-near-zero" point and extreme overestimation of modulation efficiency, and the anisotropic permittivities assumption faces problems for thickness definition and lower computational efficiency. Therefore, we treat graphene as a 2D conductive surface in the simulation to solve these problems, and investigate the plasmonic effects on modulation enhancement and the trade-off on the modulation efficiency versus the insertion loss. Our method is promising for the design of advanced optical devices based on 2D materials.

#### 1. Background

Electro-optic modulators are significant photonic devices for the link between electrical and optical signals. Compared with conventional electro-optic crystals, graphene is more promising for highperformance electro-optic modulators, which have ultra-high modulation speed, ultra-broad optical operation bandwidth, high density integration, compatibility with semiconductor technology and low costs [1,2]. However, although the optical absorption coefficient of graphene is much higher than conventional electro-optic crystals, the lightgraphene interaction for optical communication wavelengths is extremely weak due to the atomic scale of graphene thickness, which limits its further applications in electro-optic modulation [3]. Therefore, many light-trapping nanostructures for graphene have been proposed [4-6]. Recently, graphene/metal hybrid nanostructures based on plasmonic effects of metals have attracted a surge of interest [7-10]. Some plasmonic nanostructures for light trapping in graphene have been demonstrated experimentally [11,12]. Despite this, systematic design and optimization for the plasmonic nanostructures based on reliable optical modeling and compatibility with complementary metaloxide-semiconductor technology is quite in demand. In fact, graphene has an extremely small thickness and extraordinary physical properties, which bring about some new challenges in device modeling and simulation. Over the past few years, many simulation models of graphene-based electro-optic modulators have been proposed [13-

\* Corresponding authors. E-mail addresses: nanoantenna@hotmail.com (J. Zhu), qhliu@duke.edu (Q.H. Liu).

http://dx.doi.org/10.1016/j.matlet.2016.09.108

Received 20 July 2016; Received in revised form 20 September 2016; Accepted 26 September 2016 Available online 27 September 2016 0167-577X/ © 2016 Elsevier B.V. All rights reserved.

16], but these models generally treat graphene as an isotropic lossy dielectric material with a 3D bulk volume, which might lead to illusive enhancement effects of light-graphene interaction, especially for plasmonic hybrid nanostructures [17]. Recently, some researchers have realized that graphene can be considered as an anisotropic lossy dielectric material with a finite thickness due to its exceptional structural and optoelectronic properties [18], whereas the effective thicknesses of graphene for this assumption in many device models are not universal [19,20]. Therefore, it is necessary to regulate the computational assumption in the design of graphene-based electrooptic modulators. In this paper, we treat graphene as an anisotropic 2D material with a surface conductivity, and design a compact electrooptic modulator for optical intensity modulation in combination of graphene and a plasmonic nanostripe waveguide. Three simulation methods for graphene material properties are compared, and the plasmonic effects for modulation enhancement are systematically investigated.

#### 2. Methods

We design an ultra-compact modulator in combination with a gold nanostripe and a silicon waveguide on top of a buried layer of silicon dioxide, and two graphene layers are integrated on the silicon waveguide, as shown in Fig. 1. Two hexagonal boron nitride (*hBN*) layers are used as insulating layers [8]. For optical simulations, we





materials letters



Fig. 1. Design of graphene-based electro-optic modulator. The symbols w and t represent the width and thickness of the gold waveguide.

solve Maxwell's equations on a rectangularly meshed cross section of the modulator based on a finite-difference eigenmode method [21], which calculates the mode field profiles, modal effective index and propagation loss. The use of gold nanostripe makes the modulator sensitive to light polarization. The fundamental quasi-transversal electric (TE) mode is dominant, whereas the quasi-transversal magnetic (TM) mode is rapidly evanescent due to high damping in gold. Therefore, we focus on the study of TE mode.

As we demonstrated in previous work [22], Kubo formulas are used to calculate graphene's complex conductivity  $\sigma(\omega, \mu_c, \Gamma, T)$ , which is a function of angular frequency  $\omega$ , chemical potential  $\mu_c$ , scattering rate  $\Gamma$  and Kelvin temperature T.  $\Gamma$  and T are taken as 16.67 ps<sup>-1</sup> and 300 K, respectively. In the near-infrared regime, graphene can be assumed as a lossy dielectric material due to interband transition. Because the light-graphene interaction originates from the transport of carriers on the 2D surface, one can assume that graphene is an anisotropic dispersive material with an effective permittivity tensor, as defined in Ref. [22]. In this work, we simulate the same device by setting graphene as a 2D conductive surface, a volumetric isotropic dielectric material ( $\varepsilon$ =1- $\sigma$ /i $\omega$  $\Delta$ , where  $\Delta$  is the effective thickness of graphene), and a volumetric anisotropic dielectric material [22], respectively. Compared with the volumetric assumption for graphene, the 2D surface configuration treats graphene as a conductive plane with a zero thickness in numerical simulation, which requires much less discrete meshes surrounding graphene.

#### 3. Results and discussion

Initially, we reveal the influences of various graphene material configurations without a gold nanostripe, as shown in Fig. 2(a). It



Fig. 2. Attenuation as a function of  $\mu_c$  for various material configurations of graphene: (a) without a gold nanostripe, (b) with a gold nanostripe. The inset in (b) denotes the filed distributions at  $\mu_c$ =0.55 eV for 2D and isotropy configurations. Modal effective indexes for various material configurations: (c) real part, (d) imaginary part.

demonstrates that the assumptions of 2D surface conductivity and 3D anisotropic permittivities lead to almost identical simulation results, and the modulation depth is  $\sim 0.15 \text{ dB}/\mu\text{m}$ . The results of 3D isotropic permittivities are similar to the above mentioned results. However, the isotropic configurations have minor peaks between  $\mu_c=0.49$  eV to  $\mu_c$ =0.49 eV 0.53 eV, and the peak for graphene of 0.5 nm is larger than 0.35 nm. Both of the peak values are extremely amplified when a gold nanostripe is integrated, as shown in Fig. 2(b). The amplified peak value of 0.50 nm isotropic graphene around 0.52 eV is much higher than that of 0.35 nm isotropic graphene. In contrast, the results of 2D surface conductivity and 3D anisotropic permittivities for graphene are quite close to each other, they demonstrate lower propagation losses without any distinct peaks compared to isotropic graphene, and exhibit a modulation depth of ~0.20 dB/µm, which is actually 33.3% higher than the modulator without a gold nanostripe. These results can be further explained by the electric field distributions for  $\mu_c$ =0.52 eV in Fig. 2(b). When graphene is treated as a 2D conductive surface or an anisotropic dielectric material, the optical field is trapped and concentrated surrounding the corners and edges of the gold nanostripe due to the plasmonic near-field effect. The optical field intensity in this region is significantly enhanced, which strengthens the light-graphene interaction for various  $\mu_c$  from 0.1 to 0.6 eV. This leads to enhanced optical absorption in graphene (especially for smaller  $\mu_c$  from 0.1 to 0.3 eV) and increases the modulation depth, and it also pays the price of sacrificing optical loss in the gold. On the contrary, the electric field is basically trapped inside the graphene layers, when graphene is treated as an isotropic dielectric material. In a lot of research work,

light trapping in isotropic graphene is attributed to the so-called "epsilon-near-zero" (ENZ) point, in which the absolute value of graphene's complex permittivity approaches zero [13-20]. Around the ENZ point at about 0.52 eV, the effective refractive index  $n_{\rm eff}$  of the waveguide mode for isotropic graphene changes dramatically as shown in Fig. 2(c) and (d), whereas  $n_{\rm eff}$  changes gently around 0.52 eV for anisotropic graphene. This means the near-zero out-of-plane permittivity  $\varepsilon_{out}$  of isotropic graphene around 0.52 eV leads to dramatic light trapping inside graphene, and it also implies that  $\varepsilon_{out}$  of graphene is supposed to be tunable with  $\mu_c$ . However, the isotropic dielectric material assumption for graphene is inappropriate, because graphene is actually an atom-scale 2D material and the carriers excited by light energy only transport in the 2D plane of graphene, which determines that only the in-plane permittivity  $\varepsilon_{in}$  of graphene can be tuned with  $\mu_{c}$ . For this reason, graphene can be regarded as a 3D anisotropic dielectric material with a tunable  $\varepsilon_{in}$  and a constant  $\varepsilon_{out}$ . In spite of this, the assumption of anisotropic permittivity for graphene still requires an effective thickness of graphene with a definite value of  $\varepsilon_{out}$ . Over the past few years, diverse effective thicknesses and out-of-plane permittivities have been adopted, which have brought about new parameter uncertainty and intensive out-of-plane computational mesh in device simulations. As shown in Fig. 2(c) and (d), the  $n_{\rm eff}$  of different 3D anisotropic graphene tends to be divergent and gets close to that of 2D conductive graphene with reduction of effective thickness. In view of the physical properties of graphene, one can merely treat graphene as a 2D conductive surface in related simulation, which rigorously describes graphene and speeds the simulation significantly by reducing redun-



**Fig. 3.** (a) Attenuation as a function of  $\mu_c$  and w. (b) Modulation depth as a function of w, where t=20 nm. (c) Attenuation as a function of  $\mu_c$  and t. (d) Modulation depth as a function of t, where w=100 nm.

dant mesh consumption.

Based on the assumption of 2D conductive surface for graphene, we investigate the size effects of gold nanostripe. The on-state  $(\mu_c=0.55 \text{ eV})$  and off-state  $(\mu_c=0.25 \text{ eV})$  conditions are defined for the next discussion. As shown in Fig. 3(a) and (b), both of the modulation depth and the on-state insertion loss is enlarged by increasing w. The modulation depth for w=100 nm is up to 0.19 dB/ µm due to the plasmonic near-field enhancement on graphene, whereas the insertion loss reaches 0.09 dB/ $\mu m$  due to the inherent loss in gold. The modulation depth rises slowly as w increases from 0 nm to 100 nm, and rises dramatically as w increases from 100 nm to 200 nm. The on-state insertion loss increases sharply as w changes from 100 nm to 200 nm. In contrast, Fig. 3(c) and (d) demonstrate that both the modulation depth and the on-state insertion loss increase as t reduces. When t is very small  $(t/w \ll 1)$ , the propagation loss inside the gold waveguide is extremely large, which is attributed to the strong coupling between the modes on the metal/air interface and the metal/ dielectric interface. Most of the light energy dissipates as ohmic loss inside gold. The on-state optical loss is about 0.31 dB/ $\mu$ m for t=10 nm, whereas it is about 0.10 dB/ $\mu$ m for t=20 nm. The modulation depth and the on-state insertion loss changes slightly as t increase from 20 nm to 50 nm. Therefore, there is a trade-off between modulation depth and insertion loss in view of the fabrication technology of metal thin film and the requirements of insertion loss in device engineering.

#### 4. Conclusions

We design a novel near-infrared electro-optic modulator based graphene. The assumption of 2D conductive surface for graphene in device simulation demonstrates its material performance precisely and efficiently. The use of a plasmonic nanostripe in the graphene-based waveguide modulator leads to near-field confinement and a modulation

enhancement of 33.3%. The size of the nanostripe can be further optimized under the trade-off between modulation efficiency and insertion loss. Our method will benefit the future design of graphenebased electro-optic modulators for higher performance.

#### Acknowledgements

This work was supported by the NSFC (No. 61307042), Fujian Provincial Department of Science and Technology (No. 2015H0039) and the Fund of Central Universities (No. 20720150021).

#### References

- [1] Q. Bao, K.P. Loh, ACS Nano 6 (5) (2012) 3677-3694.
- [2] C.T. Phare, Y.H.D. Lee, J. Cardenas, M. Lipson, Nat. Photonics 9 (8) (2015) 511-514.
- [3] J. Zhu, O.H. Liu, T. Lin, Nanoscale 5 (17) (2013) 7785-7789.
- [4] X. Gan, R.J. Shiue, Y. Gao, et al., Nano Lett. 13 (2) (2013) 691-696.
- [5] W. Li, B. Chen, C. Meng, et al., Nano Lett. 14 (2) (2014) 955-959.
- [6] J. Niu, M. Luo, J. Zhu, O.H. Liu, Opt. Express 23 (4) (2015) 4539-4551.
- [7] A.N. Grigorenko, M. Polini, K.S. Novoselov, Nat. Photonics 6 (11) (2012) 749-758.
- [8] Y. Cai, J. Zhu, O.H. Liu, Appl. Phys. Lett. 106 (4) (2015) 043105. [9] H. Lu, B.P. Cumming, M. Gu, Opt. Lett. 40 (15) (2015) 3647–3650.
- [10] B.D. Thackray, P.A. Thomas, G.H. Auton, et al., Nano Lett. 15 (5) (2015) 3519-3523.
- [11] D. Ansell, I.P. Radko, Z. Han, et al., Nat. Commun. 6 (2015) 8846.
- [12] V.W. Brar, M.C. Sherrott, M.S. Jang, et al., Nat. Commun. 6 (2015) 7032.
  [13] Z. Lu, W. Zhao, J. Opt. Soc. Am. B 29 (6) (2012) 1490–1496.
- [14] J. Gosciniak, D.T.H. Tan, Sci. Rep. 3 (2013) 1897.
- [15] S. Ye, Z. Wang, L. Tang, et al., Opt. Express 22 (21) (2014) 26173-26180.
- [16] M. Kim, C.Y. Jeong, H. Heo, S. Kim, Opt. Lett. 40 (6) (2015) 871-874.
- [17] S. Lee, T.Q. Tran, M. Kim, et al., Opt. Express 23 (26) (2015) 33350-33358.
- [18] R. Hao, J. Jin, X. Wei, et al., Front. Optoelectron. 7 (3) (2014) 277-292.
- [19] J.S. Shin, J.S. Kim, J.T. Kim, J. Opt. 17 (12) (2015) 125801.
- [20] X. Yin, T. Zhang, L. Chen, X. Li, Opt. Lett. 40 (8) (2015) 1733-1736.
- [21] Z. Zhu, T.G. Brown, Opt. Express 10 (17) (2002) 853-864.
- [22] Y. Cai, J. Zhu, Q.H. Liu, et al., Opt. Express 23 (25) (2015) 32318-32328.