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A Tunable Dispersion Waveguide Based on Graphene–Silicon Lateral Slot Geometric Structure

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Abstract: The dispersion profiles of a hybrid graphene–silicon (HyGS) slot waveguide with trilayers of graphene are investigated in this paper. By tuning the bias voltage on graphene layer, the zero dispersion wavelengths (ZDW) of HyGS slot waveguide can be tailored dynamically and effectively. With small disturbed voltage (6 V), a large ZDW tuning amount (200 nm) is achieved, without the need for changing the geometric structure of the waveguide, which has been verified with numerical simulation. Moreover, the dispersion curve of HyGS slot waveguide is flat enough (group velocity dispersion slope less than 2 ps/nm²·km), in the vicinity of ZDW. This waveguide is highly beneficial to such applications as integrated optics and graphene-related active optical devices.

Index Terms: Nonlinear optics, integrated optics, dispersion, waveguides, subwavelength structures, nanostructures.

1. Introduction

Graphene, which is a 2-D substance of carbon whose atoms are bonded in a honeycomb lattice [1], [2], has emerged as a promising alternative material in optical devices and optoelectronic applications [3], especially for its complementary-symmetry metal-oxide semiconductor (CMOS) compatibility [4]. Owing to ultrahigh electron mobility and zero band gap [5]–[7], the graphene-on-silicon optoelectronic devices display an ultrahigh potential working bandwidth (up to 500 GHz) over a wide spectral region (covering the whole transparent window of silicon) [8]–[10]. In addition, graphene also has a giant nonlinear refractive index (10−7 cm²/W) in the telecommunication band [11]. Recently, it has become possible to fabricate ultrathin graphite material, consisting of only a few graphene layers [12], [13] and monolayer graphene [14], [15]. Therefore, various graphene-based-silicon photonic devices and their characteristics have been demonstrated and gained much attention in optoelectronics, communications, and nonlinear optics applications, such as graphene-on-silicon slot waveguide, plasmonic bandpass filter, waveguide integrated graphene electro-optic modulators, and so on.

The slot waveguide plays a significant role in signal processing [16], specifically for most of the optical energy confined inside the slot results in a larger impact on the waveguide effective index,
compared with the normal structure. Moreover, the graphene-on-silicon slot waveguide structure has many advantages, especially its suitability for investigating the nonlinear properties of graphene in the telecommunication band. To date, slot waveguide of different structures has been investigated theoretically and experimentally [17]–[22]. For example, Yang et al. theoretically proposed the TM mode graphene integrated horizontal slot waveguide as electro-absorption modulators [18]. The horizontal slot waveguide with a graphene multilayer structure has been numerically demonstrated by Yin et al. [19], which serves as a TE-pass polarizer. More recently, Wang’s research team proposed a graphene-on-silicon slot waveguide and a compact and high-responsivity photodetector has then been developed, in which graphene was grown on the silicon by the top layer CVD (chemical vapor deposition) [20]. The graphene-on-silicon-suspended vertical slot waveguide was proposed in [21], based on a commercial SOI (silicon-on-insulator) wafer, and then Mach-Zehnder interferometer and microring modulators were designed. Lu demonstrated a tunable and broadband optical field enhancement in the graphene-based nanoscale slot waveguide at infrared frequencies, and detailed theoretical analysis that the optical power and field intensity vary with the gap distance and the width of nanoribbons has been completed [22].

In the graphene-on-silicon slot waveguide structure, the conductivity of graphene could be tuned by varying the chemical potential of the graphene sheet via electrostatic biasing [18], [22]–[26], eventually leading to the change of its real and imaginary refractive index. When the Fermi level is beyond the half-photon energy (i.e. 2|μc| = ωℏ), no inter-band transition occurs in the graphene, greatly reducing the optical absorption. In this Fermi level region, the real part of the permittivity of graphene experiences an obvious change by tuning the Fermi level while the change in the imaginary part of the permittivity is negligible. The variation of the conductivity would impact the refractive index of graphene, which will introduce a way to tailor the ZDW of the waveguide dynamically and effectively. This will provide a flexible method of tuning optical properties or dispersion characteristics of the waveguide without changing it geometric structure, which has few discussed in detail so far; therefore, theoretical studies are necessary.

In this paper, we concentrate our interest on a tunable dispersion waveguide which supports waveguide modes in near-infrared frequency. A lateral slot waveguide of dielectric-graphene multilayer is studied. The optical conductivity of graphene is calculated by the Kubo formalism at T = 300 K, and it will change via loading different biased voltage, and then the effective index of waveguide is also modified, leading to a shift of the ZDW without changing its geometric structure.

2. Optical Conductivity of Graphene

Generally, graphene’s complex optical conductivity σg is composed of intra-band and inter-band contributions, which can be derived from the Kubo formalisms. The intra-band term σintra can be derived and simplified as [25]

\[ \sigma_{\text{intra}}(\omega, T, \Gamma, \mu_c) = -\frac{e^2 k_B T}{\pi \hbar^2} \left( \frac{\mu_c}{k_B T} + 2 \ln \left( e^{-\mu_c/k_B T} + 1 \right) \right) \]  

while for \( k_B T < < |\mu_c|, \hbar \omega \), the inter-band \( \sigma_{\text{inter}} \) can be approximated as [27]

\[ \sigma_{\text{inter}}(\omega, T, \Gamma, \mu_c) = -\frac{e^2}{4 \pi \hbar} \ln \left( \frac{2 |\mu_c| - (\omega - j2\Gamma) \hbar}{2 |\mu_c| + (\omega - j2\Gamma) \hbar} \right) \]  

where \( e \) represents the charge of the electron, \( \omega \) is the angular frequency, \( \hbar = h/2\pi \) is the reduced Planck’s constant, \( j \) is the imaginary unit, \( k_B \) is Boltzmann’s constant, \( T \) is thermodynamic temperature, \( \mu_c \) is the Fermi level or chemical potential, \( \Gamma = \frac{e^2 \hbar^2}{\mu_c} \) is a phenomenological scattering rate [26], \( \mu_c \) is the graphene’s carrier mobility, and \( v_F \approx 9.5 \times 10^5 \text{ m/s} \) represents the Fermi velocity. The \( \mu_c \) of graphene can be tuned by electric field, magnetic field and chemical doping [28]. In (1) and (2), the density of states per spin per unit cell has been introduced, therefore, the effect caused by the finite size of the graphene layer can be ignored in our conductivity model [29]. For the electric
Fig. 1. Three-dimensional distribution of the graphene permittivity as a function of wavelength and chemical potential: (a) real and (b) imaginary parts, respectively. (c) Permittivity and conductivity of graphene as a function of chemical potential for $\lambda = 1550$ nm. (d) Dependences of refractive index of graphene on the wavelength for chemical potential of $\mu_c = 0.4$ eV.

In a given field, the chemical potential $\mu_c$ can be defined as [30]

$$|\mu_c| = \hbar \nu \sqrt{\pi \eta (V_g - V_{\text{Dirac}})}$$  \hspace{1cm} (3)

where $\eta \approx 9 \times 10^{16} \text{m}^{-1} \text{V}^{-2}$ (reckoned from a capacitor model), and $V_{\text{Dirac}}$ represents the voltage offset of Dirac fermions in graphene. Expression $|V_g - V_{\text{Dirac}}|$ can be considered the biased voltage $V_{\text{biased}}$, which could modify the conductivity of graphene dynamically. In this model, we don’t consider any negative voltage value of $\mu_c$ since $\sigma$ is axisymmetric at $\mu_c = 0$.

According to (1)–(3), one can get the dielectric constant of a graphene layer as [28]:

$$\varepsilon = 1 + j \frac{\sigma}{\omega\varepsilon_0 \Delta} = 1 - \frac{\text{Im}(\sigma)}{\omega\varepsilon_0 \Delta} + j \frac{\text{Re}(\sigma)}{\omega\varepsilon_0 \Delta}$$  \hspace{1cm} (4)

where $\Delta = 0.34$ nm is the thickness of graphene layer, and $\varepsilon_0$ is the permittivity of vacuum.

Fig. 1(a) and (b) show how the real and imaginary parts of both the intra and inter-band contribute to the graphene permittivity, respectively, where $T = 300 \text{K}$, the graphene’s carrier mobility $\mu = 10,000 \text{cm}^2/\text{s}$ [1]. Fig. 1(c) plots the conductivity and permittivity of graphene at the wavelength of 1550 nm under the chemical potential changes from 0 eV to 1 eV. In Fig. 1(a) and (b), obviously, a transition occurs when $2|\mu_c| = \hbar \nu$ ($\mu_c = 0.4$ eV in Fig. 1(c)), of which the imaginary part experiences a sudden drop, and a negative peak value for the real part. This is attributed to the inter-band absorption with the chemical potential reaching the value of $|\mu_c|$. For a given $\lambda$, such as $\lambda = 1550$ nm, the dielectric constant changes from purely imaginary to real when chemical potential is from below 0.4 eV to over 0.4 eV; see Fig. 1(c). For conductivity, as
shown in Fig. 1(c), real ($\sigma$) shows a similar trend with the imaginary part of permittivity $\varepsilon$ under fixed wavelength, when $\mu_c > 0.4$ eV, real ($\sigma$) stays around the universal value, i.e., $\pi \varepsilon \hbar^2 / 2h \approx 0.06085$ mS/m; when $\mu_c < 0.4$ eV, real ($\sigma$) is relatively high. For the imaginary part, a positive peak value appears at the threshold chemical potential $|\mu_c|$. Fig. 1(d) display the refractive index of graphene with respect to the wavelength at $\mu_c = 0.4$ eV. As Fig. 1(d) shows, a substantial change can be observed at $\lambda = 1550$ nm, where the imaginary part of the refractive index of graphene abruptly forms a sharp peak as the wavelength varies only by dozens of nanometers, then rapidly falls to zero. Meanwhile, the real part is almost zero within the region, which implies that a drastic vibration would be caused to the effective index of waveguide. As a consequence, a destruction of the dispersion of this region is generated, which is electro-absorption, detrimental for wave propagation. In most dispersion analysis, a flat dispersion curve is generally required. Therefore, in our simulation, to avert the dramatical change of the graphene refractive index, the biased voltage is controlled to guarantee that the real part of the refractive index increases steadily with wavelength, which is very beneficial to dispersion management of waveguide. In our model, the range of the chemical potential $0.66$ eV $< \mu_c < 1.05$ eV is selected through many simulations.

3. Graphene Silicon Waveguide

Fig. 2 shows the geometrical configuration of the graphene-on-silicon lateral slot waveguide of our device mode, and the view of 3D and 2D cross section are displayed in Fig. 2(a) and (b), respectively. An 87-nm-thick $\text{Si}_3\text{N}_4$ is medially inserted in the silicon to form a lateral slot waveguide, whose width is 600 nm, and then the three layers of graphene sheet are placed at the top, bottom and center of the $\text{Si}_3\text{N}_4$, and $\text{SiO}_2$ with the width 800 nm and height 900 nm is selected as overcladding. This structure is similar to those of the ones in [17], [18]. In Fig. 2, capacitor structures are formed between the second graphene layer and the first and third graphene layers by means of the metal electrodes which are brought into contact with the graphene.

The manufacturing of this graphene-on-silicon lateral slot waveguide, which is not considered in this paper, is a separate technical issue, and the fabricated device of this structure shown as in Fig. 2 can be conducted through a series of standard methods of semiconductor fabrication in the following procedure. The bottom of the silicon layer is fabricated via the SOI process.
graphene sheet is grown by the CVD method and transferred mechanically onto the waveguide [31]–[33]. The stack of graphene and Si₃N₄ is deposited by using of (plasma-enhanced chemical vapor deposition (PECVD)) process [34]. The top of the silicon layer is planted by an orientated growth or bonding technique. By depositing a platinum film onto the graphene and connecting it to the gold pad, electrodes will be connected to the graphene [17], [30]. The undesired graphene will be removed by oxygen plasma [18], [31].

As mentioned in the previous section, since the effective permittivity of graphene appears as functions of the biased voltages, the propagation characteristics of the waveguide, such as the dispersion properties, can be tuned by applying a suitable voltage to alter the chemical potential. In order to explore how these parameters change in terms of chemical potential and wavelength, a complete description is established via using numerical and mode solving techniques in the next section.

4. The Dispersion of Waveguide

In this section, we investigate the dispersion properties of the proposed structure by numerical analysis with COMSOL MULTIPHYSICS based on finite element method. All materials involved are assumed to be nonmagnetic (μᵣ = 1) and the environment is free of external magnetic fields. The waveguide mode profiles of different mode orders are calculated with wavelength λ = 1550 nm, the chemical potential μc = 0.75 eV. Fig. 3(a) and (b) show the field distribution for the TM and TE mode, respectively. You can see that much more energy is confined inside the slot for TM mode (60.12%), comparing with the TE mode (44.62%), indicating strong interaction between light and waveguide, which would sequentially enhance the nonlinear effect and offer a more suitable condition for further study.

Fig. 3(c) displays the graphene’s index as a function of the wavelength under different chemical potentials, in which for the real part of refractive index, the solid and the dot-dashed lines stand for μc = 0.69 eV and μc = 0.95 eV, respectively, for the imaginary part, the values tend to be zero regardless of μc = 0.69 eV and 0.95 eV, which implies a poorer absorption. We focus our interest on the region marked with the two red lines, of which the working wavelength corresponds to communication band, what’s more, the real refractive index of graphene increases monotonically with the wavelength. The monotonic increased area of the real refractive index with the wavelength varies with μc. When μc is small, the wavelength start point of the monotonic increased region shifts towards the direction of long wavelength, otherwise towards the direction of short wavelength as μc is large (here the wavelength start point we call refers to the position where the imaginary part rapidly falls to zero, and the real part increases steadily with the increased wavelength at the beginning, as shown in Fig. 1(d)). For μc = 0.95, 0.69 and 0.4 eV, the location of the start point from left to right is one of the μc = 0.95, 0.69, and 0.4 eV; see Fig. 1(d) and 3(c). Because the effective index of waveguide is closely linked to refractive index of graphene, the region is one of in which the effective index of waveguide nₑₒ increases monotonically with the wavelength. Considering the relationship between effective index nₑₒ and group velocity dispersion Dλ which is

\[ D_\lambda = -\frac{\lambda}{c} \frac{d^2 n_{\text{eff}}}{d\lambda^2}. \]  

(5)

From (5), one can see that the dispersion properties of the waveguide can be tuned by varying the chemical potential of the graphene sheets via biased voltages, which may provide a robust and flexible method to change the dispersion characteristics of the waveguide and the optical properties of waveguide modes without changing its geometric structure.

Here, we explore the dispersion curve for the case of the same voltage on the three layers of graphene sheet. By applying ε (see (4)), the nₑₒ of the waveguide is simulated by COMSOL, after combining with (5), the Dλ of this waveguide can be achieved. Fig. 4(a) shows the dispersion curve under the different chemical potentials, and the corresponding different parts in Fig. 4(a) are displayed in Fig. 4(b) and (c), respectively. It can be noted that the chemical potential is tuned via loading the same voltage on the three graphene sheet layers. The two red solid horizon lines are
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Fig. 3. Optical mode profile in the waveguide for (a) TM mode and (b) TE mode at $\lambda = 1550$ nm. (c) Comparison of the refractive index of graphene under different chemical potentials. The temperature is $T = 300$ K.

$$D'_{\lambda} = \pm 100 \text{ ps/nm} \cdot \text{km}.$$ In this working region, a curve is deemed to be flat only if its absolute value of $D_{\lambda}$ is less than $D'_{\lambda}$. The value of $D'_{\lambda}$, of course, could be tuned downward to guarantee a flatter curve when $D_{\lambda}$ has a stricter limitation. However, this implies that the range of ZDW will shrink. From Fig. 4(b) and (c), one can see that by altering the chemical potential from 0.67 eV to 1.05 eV rather than transforming the geometric structure, the ZDW varies from 1451 nm to 1554.4 nm and 1654 nm to 1603 nm, respectively.

We further investigate the dependence of the zero dispersion wavelengths (ZDW) on the chemical potential. The open circles in Fig. 5(a) and (b) represent the value directly obtained with COMSOL. The curve in Fig. 5(a) is fitted by least square to describe the relation between $\mu_c$ and $\lambda$. As it shown in Fig. 5(a), the dash and solid line represent the ZDW on the left $\lambda_L$ and right $\lambda_R$, respectively. Increasing the chemical potential, the ZDW, $\lambda_L$ and $\lambda_R$, shift towards the middle, and the maximum value of the dispersion curve declines. Obviously, when the maximum value is below zero, there are no longer ZDW; therefore, the chemical potential cannot exceed 1.05 eV in our waveguide structure. The optimum parameter of the ZDW obtained is that chemical potential $\mu_c$ are from 0.67 eV to 1.05 eV, and the corresponding biased voltages are from 4.0597 V to 9.9706 V by using (3). Fig. 5(b) shows the maximum value of the dispersion curve of Fig. 4(a). This curve is beneficial to choosing the range of chemical potential on different occasions.

In addition, it is also of interest to study the thickness effect of Si$_3$N$_4$ layer. As shown in Fig. 6, the dispersion curve $D_{\lambda}$ shifts downward with thickness increased for the same chemical potential,
The entire curve shift down with the chemical potential increased. The detailed view of (b) curve in wavelength range 1435 nm–1580 nm and (c) curve in wavelength range 1605 nm–1690 nm, respectively. The zero dispersion wavelength shifts towards the longer wavelength at the left side with the chemical potential increased. On the contrary, the right shifts towards the shorter wavelength.

Fig. 5. (a) Variation of the zero dispersion wavelengths in the waveguide under different chemical potentials. (b) Maximum of dispersion curve. Both of them are calculated fitted by least square, and the open circle represents value analyzed with COMSOL.
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downward with chemical potential increased for the same thickness of Si$_3$N$_4$ layer. The dispersion curve $D_\lambda$ is below zero value as the thickness increases to 97 nm and the chemical potential is about 0.75 eV. In Fig. 4, the ZDW will no longer exist as chemical potential exceeds 1.05 eV. Consequently, curve shifting downward, which is caused by changing the geometric structure (here refers to grow the thickness of Si$_3$N$_4$ layer), means that the maximum of chemical potential will decline, which implies fewer ZDW and lower value of $D_\lambda$, but $D_\lambda$ becomes much flatter.

5. Conclusion

In this paper, we have proposed a lateral slot waveguide based on three layers of graphene to control the ZDW. By altering the external biased voltage, the effective mode index of waveguide can be modified. Consequently, the ZDW are tuned dynamically. Numerical simulation has revealed that two ZDW could shift almost in total 200 nm in our work with only 6 V changes of the biased voltage, and the dynamic range of ZDW can also be adjusted by means of the biased voltages on the graphene layers. In conclusion, the dielectric-graphene-dielectric waveguide provides a robust and simple method to achieve tunable ZDW only by changing the biased voltage. It will have promising applications in nonlinear optics and integrated optical device development for its fine optical properties.

References


