Study on properties of plasmonic waveguide of graphene-coated nanotube with a dielectric substrate

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Abstract
A hybrid plasmonic waveguide structure composed of graphene-coated nanotube with a dielectric substrate is proposed in this paper. Transmission properties of the fundamental mode are studied by the finite element method (FEM). The results reveal that the mode transmission properties are greatly dependent on the nanotube radius and internal–external diameter ratio, gap distance, nanotube permittivity, as well as chemical potential of graphene. Meanwhile, it is compared with the graphene-coated nanowires with a dielectric substrate (Hajati and Hajati in Plasmonics, 2018. https://doi.org/10.1007/s11468-017-0524-2). By optimizing the parameters, the structure could achieve long-range propagation with the propagation length about 12.56 μm. Moreover, it could realize deep-subwavelength confinement with the normalized mode area only ~10⁻⁷ in the mid-infrared (mid-IR). This structure may offer a certain theoretical basis for integrated nanophotonic devices to achieve long-distance transmission in the deep-subwavelength range.

Keywords Waveguides · Graphene · Surface plasmons · Transmission properties

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1 Introduction
Surface plasmons (SPs) (Gramotnev and Bozhevolnyi 2010; Li 2019; Liu et al. 2011) are the surface electromagnetic wave propagating at the interface between a metal and a dielectric. Because of breaking through the diffraction limit and controlling light at subwavelength scale, SPs have attracted extensive attention of scholars worldwide and developed rapidly (Roszkiewicz and Nasalski 2012; Heiss et al. 2013; Dolores-Calzadilla et al. 2015; Lu et al. 2016a; Teng et al. 2019). Usually, noble metals are used to stimulate and support surface plasmons (SPs). Various metal-based SPs waveguides
have been proposed (Berini 1999; Wang et al. 2012; Wei et al. 2018; Pile and Ogawa 2005; Veronis and Fan 2005; Moreno et al. 2008; Tanaka and Tanaka 2003; Chen et al. 2017; Bozhevolnyi et al. 2005; Lee et al. 2007; Reinhardt et al. 2006; Chen and Vladimir 2015; Shao et al. 2016; Oulton et al. 2008; Bian et al. 2009). However, the metal-based SPs waveguides usually suffer from large ohmic loss and weak field confinement in the mid-infrared (mid-IR) to terahertz (THz) frequency range (Gao and Shadrivov 2016).

Recently, it has been found that graphene can exhibit “metal-like” properties in mid-infrared (mid-IR) to terahertz (THz) wavelengths (Vakil and Engheta 2011), which can stimulate SPs. Compared to metal SPs, graphene SPs have the advantages of low propagation loss, tight field confinement and tunable electromagnetic properties (Wang et al. 2008; Koppens et al. 2011). Therefore, a large number of graphene SPs devices have been proposed, such as graphene nanoribbon waveguide (Lu et al. 2016b; Ooi et al. 2013), graphene nanowire waveguide (He et al. 2014; Wu et al. 2014), slot/wedge waveguide (Liu et al. 2013), hybrid waveguide (Sheng et al. 2016; Sun et al. 2019), and modulator (Li et al. 2014, 2018). Among them, the hybrid waveguide has a better trade-off between strong field confinement and low propagation loss, which has been widely studied in recent years. The graphene-coated nanowire waveguide (Gao et al. 2014; Yang et al. 2015; Liu et al. 2016; Hajati and Hajati 2018; Teng et al. 2020; Wu et al. 2018; Nikitin et al. 2011) is a research hotspot in hybrid waveguides because of its simple structure, easy fabrication and no cut-off of fundamental mode. It has been shown that the graphene-coated nanowire waveguide has stronger field confinement than the metal nanowire waveguide, and the normalized mode area is about $10^{-3}$ (Gao et al. 2014). In order to further improve the field confinement and reduce the mode propagation loss, researchers have proposed a graphene-based cylindrical hybrid waveguide (Yang et al. 2015; Liu et al. 2016) and the graphene-coated nanowire waveguide with dielectric substrate (Hajati and Hajati 2018; Teng et al. 2020; Wu et al. 2018). In reference Yang et al. (2015), although the normalized mode area of the graphene-based cylindrical waveguide is reduced to $10^{-6}$, the propagation distance is less than 2 μm. In reference Hajati and Hajati (2018), the propagation loss of the graphene-coated nanowire waveguides with dielectric substrate is smaller, and the propagation distance is about 7 μm. But the mode confinement is also reduced, and the mode area is one order of magnitude larger than the former.

Considering the advantages of the hybrid plasmonic waveguide, a new type of plasmonic waveguide structure composed of the graphene-coated nanotube with the dielectric substrate is designed in this paper. The main difference between the graphene-coated nanotube structure and the graphene-coated nanowire is that the nanotube is the nanostructure composed of two media, and the nanowire is pure dielectric nanostructure composed of one media. The graphene-coated nanotube waveguide structure has not been reported in related studies, and it has better performance than graphene-coated nanowire waveguide structure. The fundamental mode transmission properties of the waveguide are analyzed in detail by the finite element method. By adjusting the geometric parameters and electromagnetic parameters, the transmission properties are optimized. At the same time, the transmission properties are compared with that of the graphene-coated nanowire waveguides with the dielectric substrate (Hajati and Hajati 2018). It is found that the proposed waveguide has long propagation length and small mode area, which has important application value in the field of integrated nanophotonic devices.
2 Model and theory

Figure 1 presents a two-dimensional structural diagram of the proposed waveguide, which consists of monolayer graphene layer and dielectric nanotube as well as rectangle dielectric substrate. The studied structure is embedded in air. The inner and outer radii of the dielectric nanotube are $r_i$ and $r_o$ with the ratio $S_1(S_1 = r_i/r_o)$. The inner filling media and outer filling media of the nanotubes are different, and their permittivities are $\varepsilon_1$ and $\varepsilon_2$. The outer layer of the rectangular dielectric substrate is also filled with the medium $\varepsilon_2$ (with a height of $h_o$ and a width of $w_o$), and the inner layer of the rectangular dielectric substrate is filled with the medium $\varepsilon_1$ (with a height of $h_i$ and a width of $w_i$). The height/width ratio of inner and outer layers of the rectangular dielectric substrate is $S_2(S_2 = h_i/h_o = w_i/w_o)$. After a large number of experiments and numerical simulation results, it is found that the mode loss is small when the internal core filled the medium is air. Here, the interiors of nanotube and rectangular dielectric substrate are filled with air ($\varepsilon_1 = 1$). The gap height between the graphene-coated nanotube and the rectangular dielectric substrate is $g$. Graphene is wrapped in the outer layer of the dielectric nanotube. In the mid-infrared frequency range, the permittivity of graphene (Yang et al. 2015) can be calculated by the following formula:

$$\varepsilon_\text{g} = 1 + i\sigma(\omega)/(\omega\varepsilon_0\Delta)$$  \hspace{1cm} (1)

where $\Delta = 0.335$ nm is the thickness of single layer graphene (Hajati and Hajati 2018), $\omega$ is the radiation angle frequency of incident light, and $\varepsilon_0$ is the vacuum dielectric constant. $\sigma(\omega)$ is the surface conductivity of the graphene film, which can be derived from the famous Kubo’s formula (Nikitin et al. 2011; Francescato et al. 2013):

$$\sigma(\omega) = \sigma_{\text{intra}} + \sigma_{\text{inter}}$$  \hspace{1cm} (2)

$$\sigma(\omega)_{\text{intra}} = \frac{2ie^2k_B T}{\pi h^2(\omega + i\tau^{-1})} \ln \left[ 2 \cosh \frac{\mu_c}{2k_B T} \right]$$  \hspace{1cm} (3)

Fig. 1 Schematic of the plasmonic waveguide
\[
\sigma(\omega)_{\text{inter}} = \frac{e^2}{4\hbar} \left[ \frac{1}{2} + \frac{1}{\pi} \tan^{-1}\left( \frac{\hbar \omega - 2\mu_c}{2k_B T} \right) \right] - \frac{i}{2\pi} \ln \frac{(\hbar \omega + 2\mu_c)^2}{(\hbar \omega - 2\mu_c)^2 + 4(k_B T)^2}
\]  

where \( \sigma(\omega)_{\text{intra}} \) is the intraband conductivity of graphene and \( \sigma(\omega)_{\text{inter}} \) is the interband conductivity of graphene. Here, the temperature \( T = 300 \text{ K} \), the charge of the electron \( e = 1.6 \times 10^{-19} \text{C} \), the relaxation time \( \tau = 0.5 \text{ ps} \) (Hajati and Hajati 2017), \( \hbar \) is the reduced plank constant, \( k_B \) is the Boltzmann’s constant, and \( \mu_c \) is the chemical potential of graphene. It can be seen from the above formula that the conductivity of graphene changes with changing the frequency and chemical potential.

Because the waveguide structure proposed in this paper is complex, it is not easy to directly solve the wave equation to calculate the mode properties. Therefore, the COMSOL Multiphysics software based on the finite element method is used to calculate the mode transmission properties of the waveguide. In the process of numerical simulation, graphene is treated as an ultra-thin film with surface conductivity of \( \sigma(\omega) \). The effective refractive index is defined as \( n_{\text{eff}} = \beta/k_0 \), where \( \beta \) is the propagation constant which can be obtained directly by COMSOL software and \( k_0 \) is the wavenumber in free space; the propagation length \( L_m \) can be defined by \( L_m = \lambda_0/(2\pi*\text{Im}(n_{\text{eff}})) \), where \( \lambda_0 \) is the vacuum wavelength and \( \text{Im}(n_{\text{eff}}) \) is the imaginary part of the effective refractive index. The normalized mode area is defined as \( A_{\text{eff}}/A_0 \), where \( A_0 = \lambda_0^2/4 \) is the diffraction limit mode area and the effective mode area \( A_{\text{eff}} \), which reflects the mode confinement ability of waveguide, is defined as:

\[
A_{\text{eff}} = \int W(r) d^2r / \text{max}[W(r)]
\]

where \( W(r) \) is the electromagnetic field energy density and \( \text{max}[W(r)] \) is the maximum of electromagnetic field energy density (Wang et al. 2012; Oulton et al. 2008). Here, \( \text{max}[W(r)] \) is mainly taken in the gap between the graphene-coated nanotube and the rectangular dielectric substrate. In order to better describe the relationship between the mode propagation length and the normalized mode area, the figure of merit is defined as \( \text{FOM} = \text{Re}(n_{\text{eff}})/\text{Im}(n_{\text{eff}}) \) (Berini 2006).

### 3 Results and discussion

Figure 2a–f show the mode profiles of the electric field \(|E|\) of the fundamental mode of the waveguide structure when the air core size in the nanotube/dielectric substrate and the gap height between the nanotube and dielectric substrate are different. Here, the parameters are \( f_0 = 30 \text{ THz}, \mu_c = 0.5 \text{ eV}, w_o = 200 \text{ nm}, h_o = 100 \text{ nm}, r_o = 30 \text{ nm}, \varepsilon_1 = 1, \varepsilon_2 = 2.09 \). Meanwhile, when \( S_1 = S_2 = 0 \), the waveguide structure is similar to the structure proposed in reference (Hajati and Hajati 2018). It can be seen from Fig. 2 that most of the electromagnetic energy is confined to the gap between the nanotube and the dielectric substrate, and the mode field confinement is very strong. As the air core size increases, the electromagnetic energy gradually diffuses from the gap between the nanotube and the dielectric substrate to the periphery of the nanotube, which will lead to weak mode field confinement and low mode propagation loss. In addition, it can be seen that with the increase of gap height \( g \), the size of electromagnetic field distributed in the gap will increase, and the mode area will also increase. However, the propagation loss decreases with increasing \( g \).
The dependences of the mode properties on the ratio $S_1$ are shown in Fig. 3 under different $S_2$. As shown in Fig. 3a, when $S_2$ is fixed, the effective mode index $\text{Re}(n_{\text{eff}})$ decreases slowly with increasing $S_1$. As $S_1$ increases, the propagation length $L_m$ increases monotonically, and the normalized mode field area $A_{\text{eff}}/A_0$ also increases monotonically, but the variation range is very small. Since the propagation length increases faster than the normalized mode area, the figure of merit increases slowly. At the same time, it can be seen that when $S_1$ is small, the change of mode properties is slow, but when $S_1$ is large, the change of mode properties is fast. This is because when $S_1$ is large, the electromagnetic field will diffuse to the dielectric layer around the nanotube, the mode confinement becomes worse, and the mode loss decreases faster. That is to say, when $S_2 = 0, 0.3$, the change of mode properties is close; when $S_2 = 0.6$, $0.9$, the change of mode properties is large.

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**Fig. 2** Normalized electric field mode distributions of the fundamental mode. a $g = 5$ nm, $S_1 = S_2 = 0$; b $g = 5$ nm, $S_1 = S_2 = 0.4$; c $g = 5$ nm, $S_1 = S_2 = 0.8$; d $g = 15$ nm, $S_1 = S_2 = 0$; e $g = 15$ nm, $S_1 = S_2 = 0.4$; f $g = 15$ nm, $S_1 = S_2 = 0.8$

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**Fig. 3** Dependence of modal properties on $S_1$. a Effective mode index $\text{Re}(n_{\text{eff}})$; b Propagation length $L_m$; c Normalized mode area $A_{\text{eff}}/A_0$; d Figure of merit FOM. Here, $f_0 = 30$ THz, $\mu = 0.5$ eV, $\varepsilon_1 = 1$, $\varepsilon_2 = 2.09$, $g = 10$ nm, $r_o = 30$ nm, $w_o = 200$ nm, $h_o = 100$ nm, $S_2 = 0, 0.3, 0.6, 0.9$
0.9, the propagation length and normalized mode area change more. Especially, when \( S_1 = S_2 = 0 \), the waveguide mode properties are similar to those mentioned in reference (Hajati and Hajati 2018). It can be seen from Fig. 3 that when both \( S_1 \) and \( S_2 \) are greater than 0, the propagation length and the figure of merit of the proposed waveguide are higher than those in reference (Hajati and Hajati 2018), and the normalized mode field area does not increase much than that in reference (Hajati and Hajati 2018). Therefore, it can be said that within a certain parameter range, the mode properties of the proposed structure are better than those in reference (Hajati and Hajati 2018). For simplicity and considering the trade-off between the propagation length and normalized mode area, \( S_1 = 0.5 \) and \( S_2 = 0.6 \) are selected in the later research.

The fundamental mode properties of the waveguide structure as a function of the gap height \( g \) are depicted in Fig. 4. When \( g \) gradually increases, the coupling between graphene nanotubes and dielectric substrate decreases, resulting in the decrease of effective mode index \( \text{Re}(n_{\text{eff}}) \). Increasing the gap height leads to a larger mode area and weaker confinement. At the same time, the mode propagation loss decreases with increasing \( g \), resulting in a longer propagation length. According to Fig. 4d, FOM first increases and then tends to be flat. Therefore, the increase of \( g \) can appropriately improve the waveguide performance, but too large \( g \) has little effect on the waveguide performance. Taking into account the propagation length and the mode area, \( g = 20 \) nm is selected for the following research.

Another geometry parameter relating to the mode properties is the outer radius \( r_o \) of the nanotube. The dependences of the mode properties on parameter \( r_o \) are shown in Fig. 5, where \( r_o \) varies from 30 to 100 nm. As can be seen from Fig. 5a, \( \text{Re}(n_{\text{eff}}) \) first decreases and then increases with increasing \( r_o \). The normalized mode area increases first and then decreases with increasing \( r_o \), and the later change range is small, indicating that when \( r_o \) is large (\( r_o > 80 \) nm), \( r_o \) has little effect on the mode field confinement. Moreover, as \( r_o \) increases, both \( L_m \) and FOM gradually decrease, and the variation range is large, as shown in Fig. 4b, d. This is due to the fact that increasing the outer radius \( r_o \) of the nanotube can increase the surface area of the graphene layer, so the mode propagation loss increases and the propagation distance decreases. It can be seen from the above when \( r_o \) is the smallest, the mode properties are the best, and the figure of merit is the highest with the longest propagation length and the smallest normalized mold area. However, considering the difficulty of manufacturing, \( r_o \) should not be too small. Therefore, \( r_o = 30 \) nm is selected for the following study in this paper.

Fig. 4 Dependence of modal properties on gap height \( g \). a Effective mode index \( \text{Re}(n_{\text{eff}}) \); b Propagation length \( L_m \); c Normalized mode area \( A_{\text{eff}}/A_0 \); d Figure of merit FOM. Here, \( f_0 = 30 \) THz, \( \mu_c = 0.5 \) eV, \( \epsilon_1 = 1, \epsilon_2 = 2.09, r_o = 30 \) nm, \( w_o = 200 \) nm, \( h_o = 100 \) nm, \( S_1 = 0.5, S_2 = 0.6 \)
The permittivity $\varepsilon_2$ of nanotube/dielectric substrate also has a great influence on the waveguide performance. Figure 6 shows the dependence of the mode properties on the permittivity $\varepsilon_2$, where $\varepsilon_2$ increases from 2 to 8. In Fig. 6a, we can see that increasing $\varepsilon_2$ the effective mode index $\text{Re}(n_{\text{eff}})$ increases linearly and the mode propagation loss also increases, resulting in a smaller propagation length $L_{m}$ as shown in Fig. 6b. As can be seen in Fig. 6c, as $\varepsilon_2$ increases, the normalized mode area decreases gradually and the maximum variation range of normalized mode area is about $1 \times 10^{-7} - 6 \times 10^{-7}$, meaning that the field confinement is very tight. Figure 6d depicts the dependence of the figure of merit FOM on the permittivity $\varepsilon_2$, and it can be seen that the smaller the permittivity $\varepsilon_2$, the higher the figure of merit FOM, and the better the mode properties. Therefore, the permittivity of nanotube/dielectric substrate should be as small as possible in application. SiO$_2$ with the permittivity $\varepsilon_2 = 2.09$ is selected as the filling medium in this paper (He et al. 2013).
Compared to noble metals, the greatest advantage of the graphene is that the graphene conductivity can be dynamically tuned when its geometric structure is fixed (Wu 2018). Figure 7 shows the dependence of mode properties on frequency $f_0$ under different chemical potentials. It can be seen that as $f_0$ increases, for four different chemical potentials $\mu_c$, $\text{Re}(n_{\text{eff}})$ increases gradually, $L_m$ decreases gradually, and the normalized mode field area is complex, but it varied little. FOM gradually increases with increasing $f_0$. As can be seen from Fig. 7a, c, when $f_0$ is fixed, as $\mu_c$ increases, $\text{Re}(n_{\text{eff}})$ decreases and the normalized mode field area increases due to the weak field confinement. At the same time, as $\mu_c$ increases, the carrier relaxation time increases, which reduces the inherent loss of graphene, so $L_m$ increases, as shown in Fig. 7b. Because the propagation length increases faster than the mode field area, FOM also increases by $f_0$, as shown in Fig. 7d.

For example, when $\mu_c=0.5$ eV and $f_0=20$ THz, the propagation length and normalized mode area are 12.56 μm and $6.6 \times 10^{-7}$ respectively. Compared with the research in related fields, the proposed waveguide has the smaller normalized mold area ($\sim 10^{-7}$). In the case of the same propagation length, the normalized mode area of the waveguide proposed in this paper is two orders of magnitude smaller than that of the graphene-coated nanowire waveguide with the dielectric substrate ($\sim 10^{-5}$) (Hajati and Hajati 2018). And the normalized mold area of the waveguide proposed is one order of magnitude smaller than that of the triangular-shaped graphene-coated nanowires on substrate ($\sim 10^{-6}$) (Teng et al. 2020).

### 4 Conclusions

A graphene-coated nanotube plasmon waveguide structure with a dielectric substrate is designed and its transmission properties are studied in detail. The results have revealed that the structure proposed in this paper has better mode properties than that proposed in reference (Hajati and Hajati 2018) when the appropriate parameters are selected. The smaller the outer diameter of the nanotube, the longer the propagation length, the smaller the mode area, and the better the mode properties; meanwhile, it is shown that the waveguide structure can locally break through the restrictive relationship between surface plasmon mode
loss and mode area, that is, the mode loss and mode area are reduced at the same time. In a certain range, the larger the gap height is, the better the mode properties are. Reducing the permittivity of nanotube or increasing the chemical potential of graphene can improve the figure of merit. In particular, the proposed waveguide can realize the propagation distance in the order of ~ μm, and the normalized mode area is compressed to ~ 10^{-7}. This structure has important applications in the field of deep sub-wavelength transmission and integrated nanophotonic devices.

**Author contributions** All authors contributed to the study conception and design. Material preparation, data collection and analysis were performed by MS, ZH and LH. The first draft of the manuscript was written by MS and all authors commented on previous versions of the manuscript. All authors read and approved the final manuscript.

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**Data availability** The datasets generated during and analysed during the current study are available from the corresponding author on reasonable request.

**Declarations**

**Competing interests** Financial interests: Author Miao Sun, Zhuanling He, Xiaohong Lan and Libing Huang declare they have no financial interests. The authors have no relevant financial or non-financial interests to disclose.

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