Design of hybrid structure for fast and deep surface plasmon polariton modulation

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**Abstract:** The electric and optical performance of different surface plasmon polariton (SPP) electric modulation structures have been investigated by comparing the response speed and modulation figures of merit (FoM). To overcome the capacitance limitation and improve the response speed, we proposed a novel silver-graphene-dielectric-graphene-semiconductor vertical structure. Semiconductor nano-waveguide is introduced to help reduce ohmic loss in silver waveguide and reflect the leaked optical field back, enhancing the modulation depth. Through optimization, a device with estimated modulation FoM of more than 70% and hundreds of GHz response speed and 3 dB bandwidth is designed, which may bring great improvement to previous optical modulators.

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**References and links**

1. Introduction

Surface plasmon polariton (SPP) is a kind of electromagnetic excitation with the coupling effect of photons and electrons along the interface of materials, typically, between a metal and a dielectric [1–3]. Due to its intrinsic properties of strong field localization [4–6], SPP has huge potential applications in small and compact devices to manipulate light below diffraction limit [7]. Besides, SPP is inherently an optical field where carrier transfer is absent, therefore it has the potential to break the limit of response time that traditional electronic devices suffer from. These features make SPP-based devices promising candidates in the field of modern optoelectronic devices demanding high speed and small size, such as ultrasensitive optical sensors [8–11], ultrafast light modulators [12], and quantum information processors [13–15].

SPP modulation has been experimentally realized in metal-insulator waveguide structures [16]. It is desired to have the ability to dynamically manipulate SPPs, preferably by applying an electrical gate. One typical way is to use semiconductor layer such as silicon or ITO as the dielectric layer and apply driving voltage to change carrier density of the semiconductor to achieve SPP modulation [17,18]. However, either silicon or ITO has their constraints. Silicon based SPP modulation suffers from limited speed due to low charge carrier mobility, while...
ITO has large free-carrier absorption in telecommunication band, resulting in a low modulation efficiency.

Therefore, a better material is required for a fast and broadband modulator. Graphene, a two-dimensional material, is a good candidate in achieving electrical control of light, due to its fast carrier mobility and the low carrier scattering rate at room temperature [3,19–21]. Besides, the special linear band structure around Dirac point allows inter-band absorption modulation by tuning Fermi level [22,23], which is much more efficient compared with semiconductor charge density modulation. These properties of graphene make it a perfect fit in SPP modulator with excellent performance through both electrical [17,18,22] and optical modulation approaches [24]. Though optical modulation can achieve higher modulation bandwidth, the required optical system is complex and expensive, making it inconvenient for practical applications. Compared to optical modulation, electrical modulation is relatively easier to combine with current devices and has great potential in applications.

In our previous study, SPP’s electrical modulation based on graphene-nanowire hybrid structure has been demonstrated [22]. However, modulation speed can only go to tens of kHz limited by the device’s huge electrical capacitance, and low coupling efficiency between graphene and optical field makes modulation depth relatively small. The device design utilized in Ref [25] can realize a high modulation speed, however, optical field cannot be well confined around graphene absorber, which limits its modulation depth. To explore an optimal structure for graphene SPP modulator, we theoretically analyzed different structures and designed a novel silver-graphene-dielectric-graphene-semiconductor hybrid structure where the optical field is efficiently interacting with graphene, resulting in a higher modulation depth. More importantly, this structure allows us to get rid of the problem of huge device capacitance to enable ultrafast response of electrical modulation. By carefully selecting device parameters, our simulation results show that the response speed can reach hundreds of GHz and modulation FoM can be more than 70%.

2. Methodology

Our study is primarily based on finite element method (FEM). 2D transverse models are built to analyze optical field distribution in different structures. Besides, a 3D model for device capacitance simulation is built to acquire response time of the vertical structures. We present our results at wavelength of 700 nm, in red visible band where SPPs can be excited, propagated and easily detected in experiment. The complex refractive indexes of materials used in simulations are listed in Table 1 [26,27].

<table>
<thead>
<tr>
<th>Material</th>
<th>n</th>
<th>k</th>
</tr>
</thead>
<tbody>
<tr>
<td>Silver</td>
<td>0.051</td>
<td>4.8</td>
</tr>
<tr>
<td>Silicon</td>
<td>3.78</td>
<td>0.00257</td>
</tr>
<tr>
<td>Alumina</td>
<td>1.75</td>
<td>0</td>
</tr>
<tr>
<td>Silica</td>
<td>1.5</td>
<td>0</td>
</tr>
<tr>
<td>Cadmium Selenide</td>
<td>2.74</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 1. Values of n and k for materials in simulation.

Graphene is set as a 0.5-nm-thickness layer with relative permittivity of 2.5 [28]. Graphene conductivity is approximated by equations under 0 K temperature condition since photon energy ($h\nu$) is much bigger than $k_BT$. The calculation for graphene optical conductivity follows Eqs. (1)-(3), where $E_F$ denotes Fermi level, $e$ is electron charge constant, and $h$ is reduced Plank constant, $\sigma_{\text{intra}}$ indicates intra-band transitions in graphene, while $\sigma_{\text{inter}}$
results from inter-band transition, \( \tau \) is the relaxation time associated with intra-band transitions, \( \hbar \omega \) is photon energy. Inter-band transition of graphene can be modulated by tuning its Fermi level. As shown in Eq. (4), optical conductivity of graphene differs under two states (OFF state with inter-band transition being allowed and ON state with inter-band transition being blocked, corresponding to \( \hbar \omega > 2E_f \) and \( \hbar \omega \leq 2E_f \) respectively).

\[
\sigma = \sigma_{\text{intra}} + \sigma_{\text{inter}}
\]

\[
\sigma_{\text{intra}} = \frac{i e^2 |E_f|^2}{2\pi^2 \hbar (\omega + i\tau^{-1})}
\]

\[
\sigma_{\text{inter}} = \frac{e^2}{4\hbar} \left\{ \theta(\hbar \omega - 2E_f) - \frac{i}{2\pi} \ln \left[ \frac{(\hbar \omega + 2E_f)^2}{(\hbar \omega - 2E_f)^2} \right] \right\}
\]

\[
\theta(\hbar \omega - 2E_f) = \begin{cases} 1, & \hbar \omega > 2E_f \\ 0, & \hbar \omega \leq 2E_f \end{cases}
\]

We simulated the optical field distributions of each structure under ON/OFF states and got corresponding effective complex mode indexes, of which the real part (\( n_{\text{eff}} \)) determines propagation constant (\( \beta \)) and the imaginary part (\( \kappa_{\text{eff}} \)) is directly correlated with absorption coefficient (\( \alpha \)), shown in Eqs. (5)-(7) [1].

\[
\bar{n}_{\text{eff}} = n_{\text{eff}} - i\kappa_{\text{eff}}
\]

\[
\beta = \frac{2\pi n_{\text{eff}}}{\lambda}
\]

\[
\alpha = \frac{2\kappa_{\text{eff}} \omega}{c} = \frac{4\pi \kappa_{\text{eff}}}{\lambda_0}
\]

To analyze the influence of electrical modulation on effective absorption coefficient of the hybrid structure, modulation figure of merit (FoM) is adopted and defined as Eq. (8), where \( \alpha_{\text{ON}} \) and \( \alpha_{\text{OFF}} \) are absorption coefficients under ON and OFF states [18].

\[
\text{FoM} = \left| \frac{\alpha_{\text{OFF}} - \alpha_{\text{ON}}}{\alpha_{\text{OFF}}} \right|
\]

Since only tangential electric components interact with graphene, we use parameter \( \Gamma \) to quantify the coupling efficiency between transverse optical field and graphene [29]. \( \Gamma \) is defined by Eq. (9), where the numerator is the integration of transverse field intensity over graphene layer, and the denominator represents integrated electrical field intensity over entire simulation region.

\[
\Gamma = \frac{\iint_{\text{graphene}} (E_x^2 + E_\perp^2) ds}{\iint_{\text{total}} E_\perp^2 ds} \times 100\%
\]

### 3. Basic structure

In the basic structure, which is the same as the structure proposed by Ho et al. [29] [Fig. 1(a)], silicon substrate is coated with a thin alumina layer, then a mono-layer graphene and a silver waveguide are successively stacked on the alumina layer. Here rectangular silver waveguide is chosen for it can realize better modulation effect than cylindrical wire per unit length. Combining simulation results [Fig. 1(g)] and experiment experiences, silver waveguide is set
as 150 nm in width and 100 nm in height, which is also used in the following structures unless specifically indicated. High refractive index dielectric material alumina is chosen to increase modes refractive index, thus reducing optical leakage into silicon substrate.

Since all materials in the model have an influence on mode distribution, when alumina layer’s thickness and silver waveguide’s width is larger, optical field would be more strongly confined around the interface between alumina layer and silver waveguide, the influence of silicon substrate on optical field will decrease. As a result, the real part of complex effective mode index decreases with increasing thickness of alumina and width of silver waveguide, which leads to leakage of optical field into alumina layer and silicon substrate. As a result, coupling efficiency of optical field parallel components to graphene decreases with the increase of alumina’s thickness and silver waveguide’s width [Figs. 1(f) and 1(g)].

Distributions of fundamental mode in the basic structure are shown in Figs. 1(b)-1(e), most field energy is in vertically polarized field (Ey) confined in graphene and alumina layer, which will not interact with graphene effectively, while tangential component Ex exists only at the edge and Ez on the surface of silver waveguide. The dependence of FoM with thickness of alumina layer [Fig. 1(f)] suggests that modulation FoM can maintain a relatively high level when the thickness of alumina layer is less than 7 nm. After a sharp decrease, the modulation FoM stays at a low level. Meanwhile, the width of silver waveguide does not have much influence on modulation depth [Fig. 1(g)]. And similar variation trend of modulation FoM with that of Γ indicates that tangential components of optical field are crucial for modulation.
Signal extinction per unit length can be defined as Eq. (10).

\[ E = -\frac{10}{L} \log_{10}\left(\frac{P_o}{P_i}\right) = 8.68\alpha \]  

(10)

where \( L \) is propagation length, \( P_i \) represents input optical power, \( P_o \) represents output optical power with a propagation length \( L \), \( \alpha \) is absorption coefficient [18]. When thickness of alumina layer is 7 nm, \( n_{\text{eff}} = 3.7266 - 0.0089518i \) under ON state, extinction loss \( E_{\text{ON}} = 1.39 \) dB/\( \mu \)m, propagation length \( L_{\text{ON}} = 3.11 \) \( \mu \)m. While under OFF state, \( n_{\text{eff}} = 3.7303 - 0.033104i \), extinction loss \( E_{\text{OFF}} = 5.15 \) dB/\( \mu \)m, propagation length \( L_{\text{OFF}} = 0.84 \) \( \mu \)m.

In graphene modulation devices, modulation speed is restricted not by carrier transition time but the RC time constant of driving circuit [30,31], and their response frequency can be estimated as \( f = 1/(2\pi RC) \). In the case of basic structure, electric field can only be applied between the bottom silicon substrate and the top mono-layer graphene [Fig. 1(a)], and its capacitance can be estimated by plate capacitor equation:

\[ C = \frac{\varepsilon_0 \varepsilon_r S}{d} \]  

(11)

S is the face-to-face region between top and bottom electrodes, determined by top electrode area, including the area of mono-layer graphene, metal electrode and silver paste for connection of electrodes and metal wires, which is relatively large, up to square millimeter. At the same time, the thickness of alumina (\( d \)) can only be set as several nanometers for effective modulation. Both of these result in large device capacitance and low response speed. For example, when \( d = 7 \) nm, \( S = 0.1 \) \( \text{mm}^2 \) and resistance of the total system is 600 \( \Omega \) [31], the response speed is only about 0.232 MHz, corresponding 3dB bandwidth is 0.25 MHz. In addition, the thin large area alumina layer is easy to be punctured when high voltage is applied considering the defect density of experimental fabricated alumina.

According to our previous work, dual-confinement effect of carrier density and electromagnetic energy around the vicinity of silver waveguide will increase Fermi level shifting and decrease the actual voltage needed to tune optical transitions [22]. Through calculation, when thickness of alumina layer is about 7 nm, carrier concentration can reach \( 6.8 \times 10^{18} \) m\(^{-2} \) after applying voltages no larger than 4 V, which leads to 0.85 eV shift of Fermi level. A shift of 0.85 eV Fermi level is enough to tune optical transitions, and the corresponding electric field is lower than the breakdown field of alumina layer. When graphene is considered at room temperature, inter-band absorption change with modulation voltage is not a cut-off step, but a gradual change around 0.85eV. In this transient state, modulation depth will be smaller since the inter-band transition is only partially blocked. However, since this state is much smaller than required Fermi level, a little higher modulation over the cut-off line of 0.85eV will get over this transition state.

4. Parallel structure

To improve the optical and electric modulation performance of the devices, a structure with two parallel silver waveguides placed on the mono-layer graphene is designed [Fig. 2(a)], which is similar to the double strips structure proposed by Ho et al. [29]. As the thickness of alumina layer increases from 1 nm to 10 nm, more optical field would be leaked into the substrate. But, when the thickness of alumina layer is larger than 10 nm, the effect of silicon substrate on optical field decreases because of the confinement of optical field in the gap region [Figs. 2(b)-2(e)], which will prevent optical field from leaking into alumina layer and silicon substrate. Figure 2(f) shows the relations of \( \Gamma \) and modulation FoM with the thickness of alumina layer, both of which first drop sharply and then bounce back, finally maintaining almost unchanged after the thickness of alumina layer is larger than 150 nm.

Meanwhile, we investigate the device performance as a function of gap width between silver waveguides. When the thickness of alumina layer is set as 200 nm, both \( \Gamma \) and
modulation FoM experience a slowly decrease with the increase of gap width from 10 nm to 50 nm for large gap width is not good for the confinement of optical field [Fig. 2(g)]. When \( d = 150 \) nm, gap width between the two silver waveguides is 20 nm, \( \hat{n}_{\text{eff}} = 2.2293 - 0.016778i \) under ON state, the extinction loss \( E_{\text{ON}} = 2.61 \text{ dB/μm} \), propagation length \( L_{\text{ON}} = 1.66 \text{ μm} \). While under OFF state, \( \hat{n}_{\text{eff}} = 2.2436 - 0.085334i \), extinction loss \( E_{\text{OFF}} = 13.29 \text{ dB/μm} \), propagation length \( L_{\text{OFF}} = 0.33 \text{ μm} \).

As for electric response, the dielectric layer in this structure can be ten times thicker than the basic structure, meaning the capacity and electrical puncture problems can be alleviated to some degree. When the thickness of alumina is 150 nm, the needed applied voltage is less than 40V. For simple estimation, assuming \( d = 150 \) nm, \( S = 0.1 \text{ mm}^2 \), and total resistance of the system is \( 600 \) Ω, the response speed is only about 5 MHz and corresponding 3dB bandwidth is 5.01 MHz. So electronic response of this two-parallel silver waveguides structure will not get a large breakthrough, the problem of large face-to-face electrode area remains not solved for the connection of bottom electrode to silicon substrate [Fig. 2(a)].

5. Vertical structure

The bottom electrodes of the basic and parallel structure are connected to the large area silicon substrate, in that case all metal and conductive material over the dielectric layer will contribute to the capacitance, which will limit their response speed. Meanwhile, charges will accumulate in silicon substrate when voltage is applied, modulation speed of both the basic
and parallel structures would be limited by low charge carrier mobility of silicon to some extent. To overcome these limitations, a novel structure with two silver waveguides vertically arranged was designed [Fig. 3(a)]. In this structure, an alumina layer and a mono-layer graphene are sandwiched between two silver waveguides. We can connect the top electrode to graphene sheet while the bottom electrode to lower silver waveguide. Compared with the structures proposed by Lu et al. [32], direct contact of graphene with silver waveguide can help decrease the bias needed for modulation in visible band [22].

Fig. 3. Modulation properties of the vertical structure. (a) Schematic illustration of the vertical structure. Two silver waveguides are vertically aligned on the surface of a SiO₂ layer with a mono-layer graphene and an alumina layer placed between them. Two electrodes are connected with graphene sheet and the lower silver waveguide separately. (b)-(d) Distributions of fundamental mode polarized in different directions (X, Y and Z direction) under ON state (thickness of alumina layer is 30 nm). (e)-(h) Total optical field distributions of the fundamental mode under ON state, corresponding to the thicknesses of alumina layer of 30 nm, 60 nm, 90 nm and 120 nm respectively. (i) Side view of simulated electric field distribution of the vertical structure capacitor when the applying voltage difference of two electrodes is 1 V. (j) Dependence of $\Gamma$ and modulation FoM on the thickness of alumina layer obtained from optical field simulation.

The electrical characteristics of the vertical structure obtained from device capacitance simulation is presented in Fig. 3(i). The strong confinement of electric field by the face-to-face silver waveguides indicates that the effective face-to-face electrode area of this structure is mainly determined by the lateral area of the lower silver waveguide, resulting in dramatic enhancement of the response speed. For example, if the face-to-face area is 1.5 $\mu$m² (150 nm
wide and 10 µm long silver waveguide), and the thickness of the alumina layer is 150 nm, the corresponding capacitance obtained through simulation is about $1.26 \times 10^{-15}$ F. Assuming total resistance of the system is 600 Ω, response speed can hopefully reach up to 210.6 GHz, and 3dB bandwidth is about 200 GHz.

In the silver-alumina-silver structure, vertically polarized optical field is strongly localized in dielectric layer while the parallel polarized components Ex and Ez are confined at the edge and around the surface of silver waveguides separately [Figs. 3(b)-3(d)]. Since the upper and lower SPP modes on the interfaces are coupled with each other, when the thickness of alumina layer is as thin as several nanometers, optical field mainly exists in dielectric layer. With the increase of alumina layer’s thickness, coupling effect between the two SPP modes decreases, optical field could be more effectively confined around the graphene layer [Figs. 3(e)-3(h)]. Meanwhile, the opposite interface acts as a reflector for the leaked SPP waves, reflecting the leaked optical field back. Therefore, SPP waves can be more effectively modulated and the SPP modulation FoM will increase with the thickened alumina layer [Fig. 3(j)]. When the thickness of alumina layer $d = 150$ nm, $\tilde{n}_{\text{eff}} = 2.0531-0.0071008i$ under ON state, the extinction loss $E_{\text{ON}} = 1.1$ dB/µm, propagation length $L_{\text{ON}} = 3.93$ µm. While under OFF state, $\tilde{n}_{\text{eff}} = 2.0531-0.013048i$, extinction loss $E_{\text{OFF}} = 2.03$ dB/µm, propagation length $L_{\text{OFF}} = 2.14$ µm.

![Fig. 4. Modulation properties of the two mono-layer graphene structure. (a) Schematic illustration of the two mono-layer graphene structure. Two mono-layer graphene is sandwiched at interfaces between silver waveguides and alumina layer. (b) Dependence of $\Gamma$ and modulation FoM on the thickness of alumina layer for the optimized hybrid structure.](image)

Since SPP modes are effectively activated on both interfaces between silver waveguides and the alumina layer, another mono-layer graphene transferred to the lower interface will further improve modulation depth [Fig. 4(a)]. Oxygen plasma can be used to remove undesired graphene on one side of the waveguides, leaving the other side connected with corresponding metal electrode (for the top and bottom graphene layer, the leaving sides staggered with each other, only the part over and under the silver waveguide is overlapped). For a qualitative analysis, we simulated the optical and electric properties of this structure. The electric field distribution is the same with the vertical structure with one mono-layer graphene, meaning the potential to achieve response speed about hundreds of GHz. Although their optical field distributions is similar, our simulation results show the values of $\Gamma$ and modulation depth get a high promotion [Fig. 4(b)] because the additional introduced graphene will also modulate absorption. In this structure, when the thickness of alumina layer is 150 nm, under ON state, $\tilde{n}_{\text{eff}} = 2.0457-0.0069288i$, extinction loss $E_{\text{ON}} = 1.08$ dB/µm, propagation length $L_{\text{ON}} = 4.02$ µm. While under OFF state, $\tilde{n}_{\text{eff}} = 2.0458-0.019860i$, related extinction loss $E_{\text{OFF}} = 3.09$ dB/µm, and propagation length $L_{\text{OFF}} = 1.4$ µm.

6. Optimized hybrid structure

Though the vertical silver-alumina-silver structure provides a high response speed, it is hard to achieve a deep modulation depth due to strong ohmic loss in silver. To further improve
modulation depth, a silver-graphene-dielectric-graphene-semiconductor hybrid structure is designed with CdSe waveguide replacing the bottom silver waveguide in the vertical structure. We take the two mono-layer graphene structure [Fig. 5(a)], and set the width and height of CdSe waveguide as 500 nm and 150 nm separately. When the thickness of alumina layer is fixed at 30 nm, Figs. 5(b)-5(e) give optical field distribution of this hybrid structure under ON state. Then we set the thickness of alumina layer as 60 nm, 90 nm and 120 nm, and get the corresponding total fundamental mode field distributions [Figs. 5(f)-5(h)].

The optical field is the coupling modes of CdSe waveguide modes and silver-alumina SPP modes. With increase of alumina layer’s thickness, the two modes are separated gradually and SPP modes are better confined around the upper interface [Figs. 5(e)-5(h)]. Semiconductor waveguide will introduce many advantages compared with silver waveguide: it causes less absorption, and it can act as a reflector in the interface as well to decrease field leakage into substrate. After replacing the bottom silver waveguide with semiconductor waveguide, device modulation FoM get a promising promotion, reaching the values of more than 70% [Fig. 5(i)].
This structure can also perfectly work at 1550 nm communication band, the results are presented in Fig. 5(i). Beyond the analysis above, in this hybrid structure, CdSe waveguide could also work as a nano source to activate SPP modes under proper excitation condition, which may extend potential applications of this device structure to modulated SPP sources. For this structure, after setting the thickness of alumina layer as 150 nm, $\tilde{n}_{eff} = 2.0926 - 0.0010962i$ under ON state, the extinction loss $E_{ON} = 0.17$ dB/μm, propagation length $L_{ON} = 25$ μm. While under OFF state, $\tilde{n}_{eff} = 2.0531 - 0.013048i$, related extinction loss $E_{OFF} = 0.66$ dB/μm, propagation length $L_{OFF} = 6.55$ μm.

In our study, we noticed that the width of silver waveguide is critical to the hybrid structure’s performance, so we set it as a variable and swept for optimized values. $\Gamma$ and modulation FoM are plotted as functions of the width of silver waveguide at a fixed thickness of the alumina layer of 30 nm [Fig. 5(j)]. Although narrowing silver waveguide will enhance modulation effect, scales below 100 nm pose difficulty for fabrication process. Therefore silver waveguides between 100 nm and 150 nm are preferable.

In terms of electrical response speed of the silver-dielectric-semiconductor hybrid structure, semiconductor waveguide can be connected to electrode to maintain the up-down electrode structure. Both top and bottom electrodes are deposited on corresponding graphene sheets and face-to-face area can be reduced with a lateral displacement between two electrodes. Since the electric model is close to the vertical structure, the electric simulation results are nearly same as the vertical structure. Therefore, hundreds of GHz response speed and 3dB bandwidth are expected.

7. Conclusion

In conclusion, we have investigated several different silver waveguide SPP modulation structures, and compared their optical and electrical properties. A vertical structure is proposed and designed to obtain high speed and deep modulation of SPP. Further, semiconductor waveguide is introduced to avoid the large ohmic loss in silver-alumina-silver structure, enhancing modulation depth. Finally a novel vertical silver-graphene-dielectric-graphene-semiconductor hybrid structure with estimated modulation FoM of more than 70% and response speed of hundreds of GHz is proposed in simulation. Meanwhile, the proposed hybrid structure can realize effective optical field modulation with much lower optical power propagation loss. Simulations in our paper are based on 700 nm wavelength, but the wide absorption spectrum of graphene allows this structure to be applied to a wide optical band, for example, 1550 nm communication band. Recent development of graphene synthesis and transfer technique ensure the compatibility of these structures with the existing optoelectronics platform [33,34]. Our devices provide a way of fabricating ultra compact nano photonic devices and may find its applications in optical computing, optical communications [31], nanoscaled SPP sources, etc.

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