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Theoretical study of accumulation electron layers at ITO-dielectric interfaces and related nanostructures

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ABSTRACT

We present the transfer matrix method for accumulation electron layers at ITO-dielectric interfaces. Meanwhile, the optical transmission properties of related nanostructures are investigated in the visible frequencies. Our results show that the nanostructures possess band-stop property under corresponding conditions. It is observed that the performance of band-stop is critically dependent on the electron density and on the number of accumulation electron layers. In addition, the thickness of ITO layers and the condition of incident lights also influence the band-stop properties. Moreover, we find an optical switch behavior when the thickness of ITO layer is set as 5.0 nm. This work may provide means for designing tunable optical devices.

1. Introduction

For decades, many researchers devoted themselves to the study of multi-layer structures, which have promoted the development of many kinds of devices, such as electroluminescent devices [1–3] and optical filters [4,5]. Particularly, thin metal-dielectric stack has received widespread attention for possessing series of band-pass and band-stop regions, which can be tuned from ultraviolet to infrared regime [6,7]. Recently, metallic mesh grids [8] and graphene sheets [4,9] were employed in the multi-layer structures to replace the thin metal sheets, which expanded these band-pass and band-stop windows to low-terahertz and microwave bands. Though the multi-layer structures have great potential in many optical devices, it is limited by the difficulty in fabrication of ultrathin layers. Meanwhile, researchers have used electric charge accumulation to modulate the properties of materials' surfaces for ages [10–14]. This accumulation charge was confirmed to swarm within an extremely thin layer near the surfaces, which could generate ultrathin conductive layers on the surfaces [15–18]. Therefore, we propose to use this electrostatic modulation in the multi-layer structures, expecting conception of new optical devices.

In this work, we choose indium tin oxide (ITO) as the carrier modulation agent because ITO has been studied extensively. In addition, ITO has attracted widespread attention for its excellent characters in many fields, such as charge collectors [19], nanophotonic devices [20,21], epsilon-near-zero materials [22–25]. To simplify the simulation of electric charge accumulation, we choose a simple and common accumulation way: applying voltage on the ITO-dielectric structures. In this paper, we report on the transmission spectrum variation of electromagnetic waves through the ITO-dielectric structures when the surfaces of ITO are modulated by the accumulation electrons. It is found that the transmission spectra shows band-stop and many other features at suitable conditions, which are adjustable by changing the electron density and other parameters. In this regard, this multilayer structures of accumulation electron layers (AELs) may have great potential in optical filters, switches and other devices.

2. Models and theory

The structure we proposed is shown in Fig. 1. The dielectric media used are hafnium oxide (HfO_2), approximately with dielectric constant 3.9 at visible frequencies. The ITO layers, separated by dielectric layers, work as positive electrodes and negative electrodes alternatively. For positive layers, the electron density becomes quite small when we turn on the applied voltage. Since ITO is N-type semiconductor, electron concentration dominates the conductivity and hole concentration can be neglected in the ITO layers. Thus the conductivity of positive layers are ignored in this work and its refractive index is set as the same value of HfO_2. In the following calculations the thicknesses of the HfO_2 layers and positive ITO layers are set as 3 nm and 10 nm, respectively.

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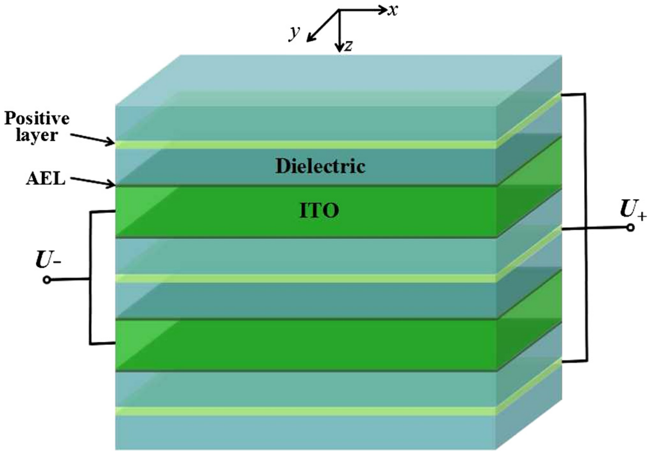

Fig. 1. Geometry of the ITO-dielectric nanostructure.

The key components in this nanostructure are the AELs, which can be characterized using theoretical models and experimental results. Refer to Drude model, the dielectric constant and conductivity of the AEL can be expressed as [17,18,26]:

$$\varepsilon_{AEL} = \varepsilon_\infty \left(1 - \frac{\omega_p^2 \tau}{\omega^2 \tau + i\omega}\right), \quad \omega_p = \sqrt{\frac{n_e e^2}{\varepsilon_\infty \varepsilon_0 m_e^*}}, \tag{1}$$

$$\sigma_{AEL}(\omega) = \frac{\sigma_0}{1 - i\omega\tau}, \quad \sigma_0 = \frac{n_e e^2 \tau}{m_e^*}, \tag{2}$$

where ω is the angular frequency of light and ω_p is plasma frequency, $\varepsilon_\infty = 3.9$ is the high-frequency dielectric constant, $\tau = 5.5 \times 10^{-15}$ s is the relaxation time of electrons, $e = 1.602 \times 10^{-19}$ C is the electron charge and $m_e^* = 3.19 \times 10^{-31}$ kg is the effective electron mass, n_e is electron density. Following previous experimental results [15,16,27], the intrinsic electron density is chosen as 5×10^{26} m^{-3}. As reported in ref [15], the electron density can be tuned from 1×10^{27} m^{-3} to 2.8×10^{28} m^{-3} under applied electric field. Considering the previous experimental results, the tunable range of electron density is chosen as 0.5×10^{27} m^{-3} to 8.6×10^{27} m^{-3} in the following calculations.

In this work, we use transfer matrix method to analyze the propagation of light through the layered media. Its main idea depends on the fact that electric and magnetic fields in one position can be correlated to those in other positions by a transfer matrix. There are two different matrices in this method: one is the transmission matrix and the other is the propagation matrix.

Transmission matrix illustrates the fields across an interface. We first consider the propagation of light across an AEL that separates two dielectrics with dielectric constants ε_1 and ε_2. Light is assumed to propagate in the z direction. In this work, s- and p-polarized lights propagate independently, so we deal with them separately. We consider the AEL lying at $z = 0$. For s-polarization, the electric field is polarized along the y direction and can be written as the form

$$E_{1y} = (a_1 e^{ik_{1z}z} + b_1 e^{-ik_{1z}z}) e^{ik_{1x}x}, \quad (z < 0), \tag{3}$$

$$E_{2y} = (a_2 e^{ik_{2z}z} + b_2 e^{-ik_{2z}z}) e^{ik_{2x}x}, \quad (z > 0). \tag{4}$$

where a_i and b_i ($i = 1,2$) are the field coefficients, a_i represents waves propagating along the z direction and b_i represents waves propagating along the -z direction, k_{ix} is the x component of the wavevector $k_i = \sqrt{\varepsilon_i}\omega/c$, and $k_{ix} = k_i \sin\theta_i$ (θ_i is the incident or refractive angle); k_{iz} is the z component of the wavevector k_i, and $k_{iz} = k_i \cos\theta_i$. Here ω is the angular frequency and c is the speed of light in vacuum. In this work, we regard all materials as nonmagnetic, i.e. with relative magnetic permeabilities $\mu = 1$.

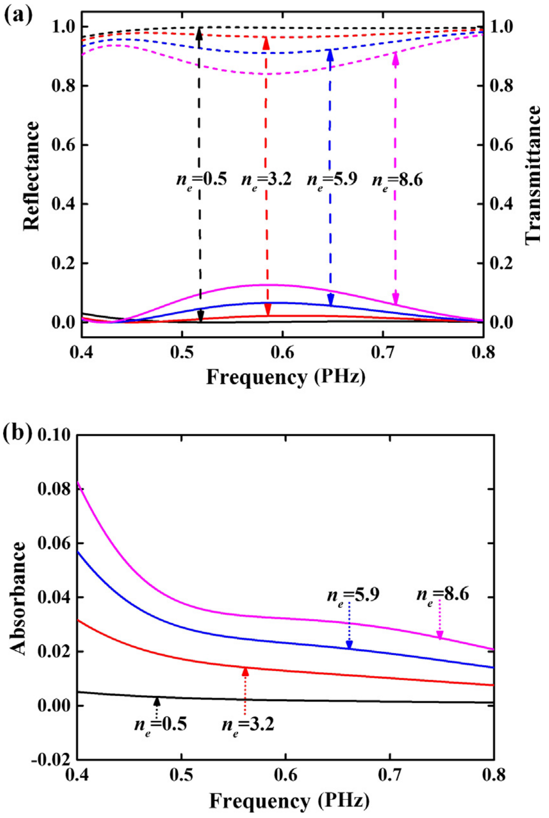

Fig. 2. (a) Reflectance (solid line), transmittance (dash line) and (b) absorbance of two-layer AEL structure at different electron density. The unit of n_e is 10^{27} m^{-3}.

Table 1
Peak (valley) values of reflectance (transmittance) at different electron density in Fig. 2(a).

n_e (10^{27} m^{-3})	Peak value	Valley value
0.5	0.004	0.995
3.2	0.023	0.964
5.9	0.066	0.911
8.6	0.127	0.841

From Snell's law $\sqrt{\varepsilon_1}\sin\theta_1 = \sqrt{\varepsilon_2}\sin\theta_2$, we know that $k_{1x} = k_{2x}$. And the electric and magnetic fields at the interface satisfy the following boundary conditions:

$$E_{1y}\big|_{z=0} = E_{2y}\big|_{z=0}, \tag{5}$$

$$H_{2x} - H_{1x}\big|_{z=0} = t_{AEL}\sigma_{AEL}E_y\big|_{z=0}, \tag{6}$$

where t_{AEL} is the thickness of the AEL and it can be estimated as 1.0 nm [15–18]. Then we obtain

$$a_1 + b_1 = a_2 + b_2, \tag{7}$$

$$\sqrt{\frac{\varepsilon_2\varepsilon_0}{\mu_0}}(-a_2 + b_2)\cos\theta_2 - \sqrt{\frac{\varepsilon_1\varepsilon_0}{\mu_0}}(-a_1 + b_1)\cos\theta_1 = t_{AEL}\sigma_{AEL}(a_1 + b_1). \tag{8}$$

Combining Eqs. (5) and (6), the coefficients a_1 and b_1 can be related to a_2 and b_2 by a transmission matrix M_s,

$$\begin{bmatrix} a_1 \\ b_1 \end{bmatrix} = M_s \begin{bmatrix} a_2 \\ b_2 \end{bmatrix}, \tag{9}$$