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Theoretical analysis of optical properties and sensing in a dual-layer asymmetric metamaterial

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Surface plasmon polaritons (SPPs) have undisputed advantages like strong enhancement of the local electric field and much better adaptability to nano architectures. Here, we propose a three-dimensional plasmonic metamaterial consist of two nanorod layers, where this system comprises two silver bars stacked above another two symmetric silver bars. We use a theoretical model, which well explains the generation of plasmon induced transparency (PIT) phenomena. The highest reflection and absorption can reach about ninety percent and forty percent by tuning the asymmetry, respectively. As one of the applications, plasmonic sensors rely either on surface plasmon polaritons or on localized surface plasmons on continuous or nanostructured noble-metal surfaces to detect many events. In the sensing devices, an important comparative parameter of sensing devices is the figure of merit (FOM), and we also demonstrate the FOM via changing the refractive index of environmental dielectric. By adjusting the parameters, we can realize a high FOM, and an interesting double-peak sensing is also obtained in this plasmonic metamaterial sensor. The proposed model and findings may provide guidance for fundamental research of the integrated plasmonic nanosensor applications.

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1. Introduction

Surface plasmon polaritons (SPPs), a very strong localized wave, can be born out of the boundary of metal and dielectric when a polarized light is irradiated. The reason is that the surface electrons of the noble metal nanostructure possess powerful active properties. SPPs have special phenomena like the high confinement and localized enhancement, so they can be applied to improve the absorption of active materials. Moreover, the optical properties of SPPs are worthy of consideration in the application. The SPPs can break the diffraction limit [1], therefore, it has aroused great interest of the researchers since its discovery and more and more relevant reports of SPPs are emerging in an endless stream. As yet, there are a lot of applications on SPPs like the optical switch [2,3], slow light devices [4–6], plasmonic waveguide filters [7,8], sensors [9,10], and various metamaterials [11–15].

Plasmon-induced transparency (PIT) is a typical destructive interference effect resulting from the strong coupling between the wide-band bright mode and the narrow-band dark mode in meta-atoms of metamaterials [16]. As an application of PIT, the metal–dielectric–metal (MDM) or metal–insulator–metal (MIM) waveguide structures have been widely studied in a large number of papers and articles since they are easily fabricated and have deep subwavelength confinement of light with an

acceptable propagation length for SPPs [17,18]. So far, the MDM waveguide structure has also been used for the sensor research [19]. But there is not much research on the three-dimensional plasmonic metamaterial sensor. In addition, a suitable theoretical model, which can be used to predict the sensing performance of structures, is not established in recent articles. We introduce coupled mode theory (CMT) to investigate the spectral responses and sensing applications in plasmonic metamaterial with multi silver bars in our paper. However, this model is always used to discuss optical properties of waveguide structures, and it is rarely used for the PIT phenomenon in plasmonic metamaterial systems. From the comparison of numerical simulation and theoretical results, we can find that the CMT model is very appropriate. Transmission and reflection spectroscopy are nowadays the most widespread techniques for the optical characterization of three dimensional metamaterial systems. Therefore, we investigate the transmission and reflection spectra about our plasmonic systems by the finite difference time domain (FDTD) method.

In this paper, we introduce coupled mode theory (CMT) to study the FOM and spectral responses in the plasmonic metamaterial system. The structure of this nano plasmonic metamaterial system is consists of two functional layers which comprise two silver bars stacked above another

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Fig. 1. (a) Schematic of the metamaterial structure. Red color represents the silver wires in the bottom layer and yellow color represents the silver bars pair in the top layer. (b) Equivalent CMT model for our proposed structure. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

two symmetric silver bars (see in Fig. 1(a)). The elements in the two layers are oriented perpendicular to each other.

2. Structure and theory model

Fig. 1(a) shows the schematic illustration of our metamaterial structure. It consists of two silver bars (in yellow) stacked above another two symmetric silver bars (in red) in a dielectric environment. The upper and lower silver bars are all on the same horizontal level, respectively. They have a vertical distance $t_{13} = t_{24} = 15$ nm , and the other fixed geometrical parameters are as follows: $t_1 = t_3 = t_2 = t_4 = 50 \text{ nm}$, $l_1 =$ $l_2 = 300 \text{ nm}, w_1 = w_2 = 80 \text{ nm}, w_{12} = 120 \text{ nm}, l_3 = l_4 = 280 \text{ nm}, w_3 = 120 \text{ nm}$ $w_4 = 100$ nm. In the following, we are going to display systematic tuning of the PIT spectra in these stacked samples by introducing structural asymmetry which is distance (w_{34}) of the upper silver bars. We first choose air as the dielectric into numerical simulation, and then in order to further combine with the experiment [12], we also introduce another dielectric whose name is glass (SiO₂). The frequency dependent permittivity of the silver is approximated by the Drude model defined as $\varepsilon(\omega) = \varepsilon_{\infty} - \omega_p^2 / (\omega^2 + i\omega\gamma_p)$ [20–22], where ω is the angular frequency of the incident wave, ε_∞ = 3.7 is the dielectric constant at the infinite frequency, $\omega_p = 1.38 \times 10^{16}$ rad/s is the plasma frequency, and $\gamma_n = 2.73 \times 10^{13}$ rad/s is the damping rate, respectively. When a wave is injected and coupled into the layers, SPPs wave forms on the metallic interfaces, and then it is confined in the gap and surface of four nano-silver bars. Fig. 1(b) demonstrates an equivalent CMT model, and the two ellipses represent two resonators for CMT model. a_n stands for the positive frequency component of the *n*th resonator mode amplitude. The resonant mode is described by $da_n/dt = i\omega_n a_n$ alone. $S_{\pm,in}^n$ and $S_{\pm,out}^n$ are expressed as the wave traveling forward (in) or backward (out) the nth resonator of amplitudes (The subscript \pm represent two propagating directions of the wave), as shown in Fig. 1(b). The characteristic spectra of our structures are simulated by the threedimensional (3D) FDTD method [23]. The spatial and temporal steps are set as $\Delta x = \Delta y = \Delta z = 5$ nm and $t = \Delta x/2c$ (*c* is the velocity of light in vacuum), respectively. We perform the FDTD simulations with a perfect matched layer boundary condition at z direction and periodic boundary conditions at x and y direction, respectively.

As the SPP waves pass through the layers, the energy can be coupled into the equivalent resonators and the dynamic transmission characteristics of our proposed structure can be investigated by the CMT [24,25]. Thus, the energy amplitude a_n of the *n*th resonator (n = 1, 2) can be expressed as

$$\frac{da_1}{dt} = \left(i\omega_1 - \frac{1}{\tau_{o1}} - \frac{1}{\tau_{e1}}\right)a_1 + S^1_{+,in}\sqrt{\frac{1}{\tau_{e1}}} + S^1_{-,in}\sqrt{\frac{1}{\tau_{e1}}} - i\mu_{12}a_2 \tag{1}$$

$$\frac{da_2}{dt} = \left(i\omega_2 - \frac{1}{\tau_{o2}} - \frac{1}{\tau_{e2}}\right)a_2 + S^2_{+,in}\sqrt{\frac{1}{\tau_{e2}}} + S^2_{-,in}\sqrt{\frac{1}{\tau_{e2}}} - i\mu_{21}a_1 \tag{2}$$

here, ω_n (n = 1, 2) is the *n*th resonant angular frequency, $1/\tau_{on} = \omega_n/(2Q_{on})$ is the decay rate due to intrinsic loss, $1/\tau_{en} = \omega_n/(2Q_{en})$ is the decay rate due to energy escaping into outside space (n = 1,

2), and $\mu_{12}(\mu_{21})$ is the coupling coefficient between the two resonant modes, respectively. Q_{on} and Q_{en} are cavity quality factors related to the intrinsic loss in *n*th resonator and the delay rate into outside space, respectively. The relationship among Q_{on} and Q_{en} for the *n*th resonator is $1/Q_{in} = 1/Q_{on} + 1/Q_{en}$, where Q_{in} is the total quality factor of the *n*th resonator in coupled system. The Q_{in} is defined as $Q_{in} = \lambda/\Delta\lambda$ (here λ is the wavelength of the peak and $\Delta\lambda$ is the full width at half maximum of the PIT windows). With the conservation of energy, they also satisfy the following relations

$$S_{+,out}^{1} = S_{+,in}^{1} - \sqrt{\frac{1}{\tau_{e1}}} a_{1}, \quad S_{-,out}^{1} = S_{-,in}^{1} - \sqrt{\frac{1}{\tau_{e1}}} a_{1}$$
(3)

$$S_{+,out}^2 = S_{+,in}^2 - \sqrt{\frac{1}{\tau_{e2}}} a_2, \quad S_{-,out}^2 = S_{-,in}^2 - \sqrt{\frac{1}{\tau_{e2}}} a_2 \tag{4}$$

From Eqs. (1)–(4), the condition that the light is only injected from the first port ($S_{-,in}^2 = 0$), $S_{+,in}^2 = S_{+,out}^1$ and $S_{-,in}^1 = S_{-,out}^2$, we can achieve the complex transmission coefficient *t* and reflection coefficient *r* of this system:

$$t = \frac{S_{+,out}^2}{S_{+,in}^1} = 1 + (\gamma_1 \gamma_2 - \chi_1 \chi_2)^{-1} \left(\chi_2 \sqrt{\frac{1}{\tau_{e1} \tau_{e2}}} - \gamma_2 \frac{1}{\tau_{e1}}\right) + (\gamma_1 \gamma_2 - \chi_1 \chi_2)^{-1} \left(\chi_1 \sqrt{\frac{1}{\tau_{e1} \tau_{e2}}} - \gamma_1 \frac{1}{\tau_{e2}}\right)$$
(5)
$$r = \frac{S_{-,out}^1}{S_{-,out}^1} = (\gamma_1 \gamma_2 - \chi_1 \chi_2)^{-1} \left(\chi_1 \sqrt{\frac{1}{\tau_{e1} \tau_{e2}}} - \gamma_1 \frac{1}{\tau_{e1}}\right)$$

$$S_{+,in}^{1} \qquad (\bigvee \tau_{e1}\tau_{e2} \quad \tau_{e2}) + (\gamma_{1}\gamma_{2} - \chi_{1}\chi_{2})^{-1} \left(\chi_{2}\sqrt{\frac{1}{\tau_{e1}\tau_{e2}}} - \gamma_{2}\frac{1}{\tau_{e1}}\right)$$
(6)

where $\gamma_1 = i\omega - i\omega_1 + 1/\tau_{e1} + 1/\tau_{e1}$, $\gamma_2 = i\omega - i\omega_2 + 1/\tau_{e2} + 1/\tau_{e2}$, and $\chi_1 = i\mu_{21} + \sqrt{1/(\tau_{e1}\tau_{e2})}$, $\chi_2 = i\mu_{12} + \sqrt{1/(\tau_{e1}\tau_{e2})}$. Thus, the transmittance $T = |t|^2$, reflectance $R = |r|^2$, and absorbance A = 1 - T - R can be obtained, respectively.

3. Results and analysis

In order to further illustrate the transmission characteristics of our proposed PIT structure, we use FDTD method to simulate spectra response. Combined with CMT, the simulative and theoretical transmittance spectra, reflectance spectra, and absorbance spectra for the structure of Fig. 1(a) with different w_{34} (10 nm–90 nm) are presented in Fig. 2(a), Fig. 3(a), and Fig. 3(b), respectively. The decay rates and the coupling coefficients obtained from theoretical calculation and the FDTD simulations are fitting parameters. For theoretical transmission spectra and structural properties of dual-layer asymmetric metamaterial, the quality factor are approximately equal to $Q_{t1} = 14$, $Q_{t2} = 11$, $Q_{o1} = 15$, and $Q_{o2} = 13$, respectively. The coupling coefficients are $\mu_{12}(\mu_{21}) = 2.5 \times 10^{13}$ rad/s, respectively. The resonant angular frequency $\omega_1(\omega_2)$ corresponding to $w_{34} = 10$, 20, 30, 40, 50, 60, 70, 80, and 90 nm are 1.920×10^{15} rad/s, 1.934×10^{15} rad/s, 1.934×10^{15} rad/s, 1.946×10^{15}

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