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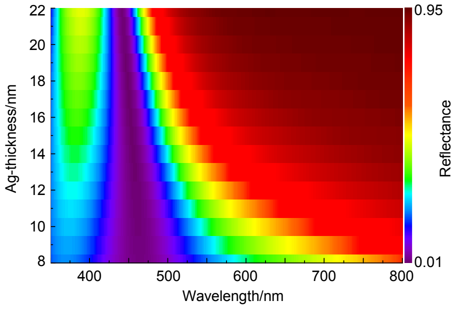
Optical characteristics of one dimensional metal-dielectric photonic band gap material



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Abstract: This paper describes the optical transmittance and reflection of one dimensional metal-dielectric photonic-band gap material (1D M-D PBG), which is made of different thicknesses ITO and Ag layers. It is found that structures with a unit size below 80 nm and a smaller metal fraction leads to improvement of optical transmittance. For unit sizes larger than 80 nm, the reflection at the shorter and longer wavelengths increases. This is due to the generation of a structural and plasmonic band gap. In addition, the reflection in both ranges increases and broadens by increasing Ag films thicknesses. The reflection spectrum induced by structure shifts towards longer wavelength as a result of unit size increasing and the reflection due to plasmonic band gap piles beyond to optical range. The results are very useful for optical filter of 1D M-D PBG design.

Keywords: metal photo crystals; optical transmittance; optical reflection

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一维金属介质光子带隙材料的光学特性

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摘要：本文描述了由不同厚度的 ITO 和 Ag 层制成的一维金属介质光子带隙材料 1D M-D PBG 的光学透射和反射特性。研究发现，单元尺寸小于 80 nm 的金属结构和较小的金属分数会导致光学透射率的提高。对于大于 80 nm 的单元尺寸，在可见光的低频和高频的频谱范围内反射率都相应增强。这是由于一种特殊结构和等离子体的带隙的作用。此外，在两个范围内的反射随着增加银膜厚度的增加而提高和扩大。结构引起的反射光谱随着单位尺寸的增大而增大，并且由于等离子体光子带隙的反射超出光学范围。研究结果对 1D M-D PBG 光学滤波器的设计有一定的参考价值。

关键词：金属光子晶体；光学透射率；光学反射

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1 Introduction

Nowadays, one-dimensional metal-dielectric photonic band gap materials (1D M-D PBG) have attracted a great attention because of their special properties [1-13]. In these structures, permittivity is a periodic function in space. Electromagnetic waves within the photonic band gap cannot propagate inside the 1D M-D PBG. Thus, the electromagnetic energy is totally reflected, and the 1D–PBG can be used as a very effective reflector for the incident wave[14-15]. Compared to dielectric-dielectric photonic band gap materials, a fewer numbers of periods would be enough to achieve photonic band gap when using M-D PBG[16-17]. In general, transmittance through a metal film is quite low and decreases exponentially with the thickness of the metal film. The low transmittance of metals limits their operating range to wavelengths near the plasma frequency (where metals are semitransparent) and metal films less than about 50 nm thick. In order to overcome these limitations of single metal films, plenty of studies have focused on the optical characteristics[18]. It is worthy to note that 1D M-D PBGs, for example, exhibit good transmittance even if the total metal thickness is much larger than its skin-depth in optical range[19-20]. Moreover, these materials can also be designed to enhance reflection[21]. Most of researches have been focused on the relation between optical transmittance and the fraction of metal. For instance, the location and bandwidth shift towards longer wavelengths and broaden by decreasing the metallic fraction[12-13]. Lots of researchers have mainly concentrated on improving optical transmittance[18-19,21]. It is well known that the high optical transmission of 1D M-D PBGs is due to resonant tunneling. However, there are two crucial factors determining optical transmittance have never been taken into account in previous work. One factor is that a structure band gap may be present in the optical structure. The other factor is that the plasmonic band gap may extend into the optical region. Both of these factors may decrease the transmittance and possibly even eliminate optical transmittance for specific wavelength ranges. Generally, this phenomenon doesn't hope to happen in designing optical windows. Here, the structure band gap is determined by the structure of 1D M-D PBG, such as the refractive index contrast, metallic fraction, and unit size. The plasmonic band gap, on the other hand, is induced by negative permittivity, which is located in the longer wavelength region starting from the wavelength whose permittivity is zero. The aim of this work is to search the mechanism how the structure and plasmonic band gap co-exist in optical region. Here, we designed 1D M-D PBG which composed of alternating layers of Ag and ITO on top of a glass substrate and studied their optical phenomena, such as transmission and reflection with different structures. Ag was chosen as the metal component because Ag-PBG exhibits better optical transmittance than other noble metal PBG (Au-PBG, Cu-PBG and Al-PBG)[22]. Additionally, Ag exhibits a negative value of permittivity in optical range. Similarly, ITO is a potential oxide dielectric material having better optical transmittance and a positive value of permittivity. Moreover, ITO films exhibit non-absorbing characteristics in optical regime. Optical performance of 1D M-D PBG with different metal fraction and unit size were simulated by mean of the finite-difference time-domain (FDTD) method[23]. The mechanisms of how the 1D M-D PBG induce structure and plasmonic band gap and further cause the optical transmittance decreasing were presented in the paper.

2 Method and model

The designed structure of 1D-MD PBG is shown in Fig.1. It consists of Ag metal layers with permittivity and thickness, and ITO layers with permittivity and thickness. Both layers are made of non-magnetic materials with permeability. The 1D M-D PBG is periodic in *z* direction and uniform in the *x* and *y* directions. In each unit, the thickness of Ag film was chosen to be below 22 nm in order to obtain a better transmittance (a thicker metal films will block light transmission). In addition, the thickness of each ITO layer was made to be below 200 nm and the number of period of 1D M-D PBG was fixed 3.5. We have found that it is enough to obtain a photonic band gap for 1D M-D PBG[24]. Here, in order to improve adhesion between substrate and metal-dielectric multilayer films and protect Ag from oxidation, ITO films were chosen as the innermost and outermost layers.

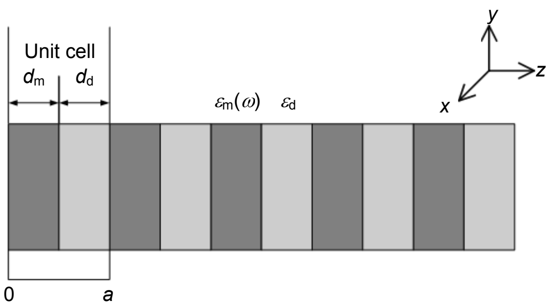

Fig. 1　Structure of the Ag-PBG with 3.5 pairs

The optical characteristics were investigated using the finite difference time domain (FDTD) method[21]. Such metallic elements were considered to have Drude dielectric function as follows[25-27]:

$$\varepsilon_{\mathrm{m}} = \varepsilon' + \varepsilon'' = \varepsilon_{\infty} - \frac{\omega_{\mathrm{p}}^2}{(\omega^2 + \Gamma^2)} + \mathrm{i}\frac{\omega_{\mathrm{p}}^2 \Gamma}{\omega(\omega^2 + \Gamma^2)} \quad , \tag{1}$$

where, ε' and ε'' represent the real and the imaginary part of the permittivity of Ag films, respectively. Where the plasmonic frequency of ω_{p}=14.0×1015 rad/s and the damping constant of Γ=0.032×1015 rad/s are obtained from the literature[25]. The empirical value ε_{∞} for silver is about 5, which is a sum or integral after taking all pertinent transitions into account[25]. Additionally, the ITO permittivity was taken as 3.13, which was measured using an ellipsometer (SENTECH SE8000dv-PV). During the process of simulation, the refractive index of substrate was approximately 1.52 for a wide optical range.

3 Results and discussions

3.1 Transmittance of Ag-PBG

The transmission spectra simulated using FDTD were presented at normal incident with ITO thickness at 60 nm and 3.5 periods. The unit size for all samples was below 80 nm. It is clearly seen that the transmittance improved and broaden with decreasing metallic fraction. This regulation agrees well with others[21]. Additionally, there is an interesting phenomenon being worthy to be mentioned that difference between the three spectra in the range from 500 nm to 780 nm are far more than that from 380 nm to 450 nm. This phenomenon is determined by two factors. One is that the difference of the spectra below 450 nm is mainly induced by the reflection of the Ag films. The reflection will be stronger as each Ag layer thickness increasing and the transmittance accordingly decreases. However, a larger difference is produced by different effective plasmonic wavelength in the range from 500 nm to 780 nm. Assuming the absorption effect can be neglected, 1D M-D PBG can be characterized using an effective dielectric function as shown in equation (2)[22].

$$\varepsilon_{\mathrm{eff}} = 1 - \frac{\Omega_{\mathrm{p}}^2}{\omega^2} \quad , \tag{2}$$

where Ω_{p} is the effective plasmonic frequency and ω is the optical frequency. $\varepsilon_{\mathrm{eff}}$ is the effective permittivity of 1D M-D PBG.

So as to that 1D-MD PBG is opaque for wavelength longer than the effective plasmonic wavelength because it behaviour as an effective medium with negative permittivity. Moreover, light with a wavelength below the plasmonic wavelength transmits well because the effective permittivity is positive and propagating modes are allowed[22]. This is the reason why the 1D M-D PBG can enhance optical transmittance.

When each the thickness of each layer is sufficiently smaller than the incident wavelength, the effective permittivity of 1D M-D PBG is a function of the ratio between metal and dielectric thickness as expressed in equation (3)[22, 28].

$$\varepsilon_{\mathrm{eff}} = \frac{\varepsilon_{\mathrm{d}} + \eta\varepsilon_{\mathrm{m}}}{1+\eta} \quad , \tag{3}$$

where, η denotes the ratio of adjacent Ag layer thickness (d_{m}) to ITO thickness (d_{d}).

$$\eta = \frac{d_{\mathrm{m}}}{d_{\mathrm{d}}} \quad . \tag{4}$$

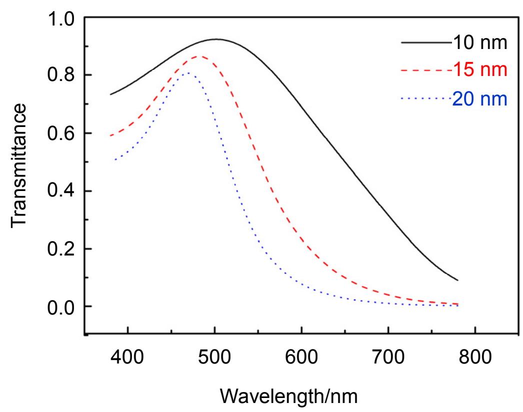

Fig. 2 Optical transmission spectra simulated using FDTD for normal incidence with 3.5 pairs of layers consisting of 10 nm, 15 nm and 20 nm Ag films respectively, and a fixed ITO films thickness at 60 nm transmittance

The equivalent permittivity was calculated by substituting ε_{m} obtained from equation (2) and ITO film permittivity into equation (3). The equivalent permittivity of 1D M-D PBG for different ratio between Ag and ITO thickness is shown in Fig. 3. It is clearly seen that the plasmonic wavelength whose equivalent permittivity is zero shifts towards longer wavelengths as η decreases. When η is lower than 1:8, the wavelength will be beyond optical region. Thus, the plasmonic band gap extends into the optical region when the metal ratio greater than 1:8. In other words, the transmission spectrum is broadened while η decreases, due to the longer plasmonic wavelength. This is the reason why optical transmission spectra broaden with η decreasing.

When η is 1:1 and 1:2, the optical transmittance is very poor and the transmission bandwidth in the optical range is narrow, as shown in Fig. 3. As the value of η decreasing, the cutoff wavelength shifts towards to longer wavelength due to longer plasmonic wavelength. As can be seen in Fig. 4, there are two peaks in the transmission spectra when the thickness of each ITO layer is greater than 60 nm. There is also a novel phenomenon: a stop band appears for samples with a unit cell of a=120 nm.

In order to further elaborate the effect of unit sizes on optical performance, the transmittance of samples with unit range 140 nm to 220 nm were also studied by

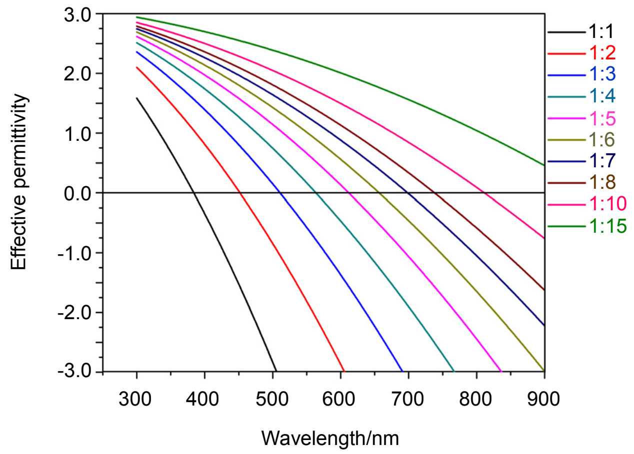

Fig. 3 Calculated effective permittivity for a ratio of Ag to ITO thickness of 1:1. 1:2,1:3 1:4, 1:5, 1:6, 1:7, 1:8, 1:10 and 1:15, according to equation (3)

FDTD. It is clearly seen that there is a stop band appears in optical range when the unit size is larger than 120 nm. As shown in Fig. 5, the plasmonic wavelength goes beyond optical range for samples with η smaller than 1:7. Therefore, the occurrence of a stop band in optical range can be attributed to a structure band. As a result, the first structure band gap is associated with the Bragg condition, as expressed in equation (5)[7].

$$\lambda = 2na \quad , \tag{5}$$

here, λ is the central wavelength of the first band gap and a is the lattice constant as shown in equation (6).

$$a = d_{\mathrm{m}} + d_{\mathrm{d}} \quad . \tag{6}$$

Furthermore, n is the effective refractive index, which can be expressed as follow[22]:

$$n = \sqrt{\varepsilon_{\mathrm{eff}}} \quad . \tag{7}$$

The value of η, the unit size a, and the effective refractive index simultaneously increase along with increasing of ITO films thickness. According to equation (5) the central wavelength of the first band gap shifts towards to longer wavelength accordingly. As shown in Table 1, the band gap significantly increases when the unit size increases in the beginning. However, the band gap changes little, and it can even be neglected as the unit size further increasing. Moreover, the central wavelength redshifts at the same time, but the increasing gradient gradually diminishes due to the effective refractive index

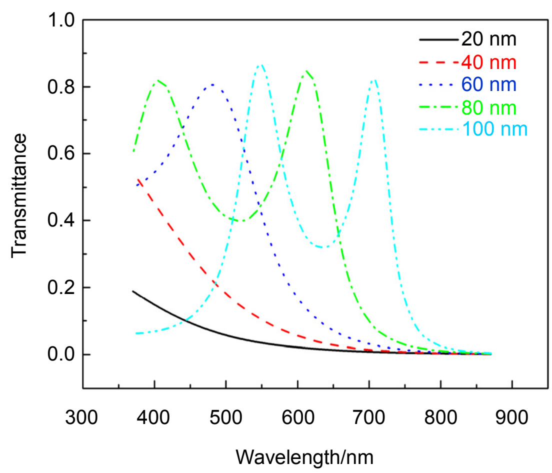

Fig. 4 Optical transmission spectra simulated using FDTD for normal incidence with 3.5 pairs of Ag/ITO, which consist of 20 nm, 40 nm, 60 nm, 80 nm and 100 nm ITO films, respectively, and fixed Ag films of 20 nm thickness

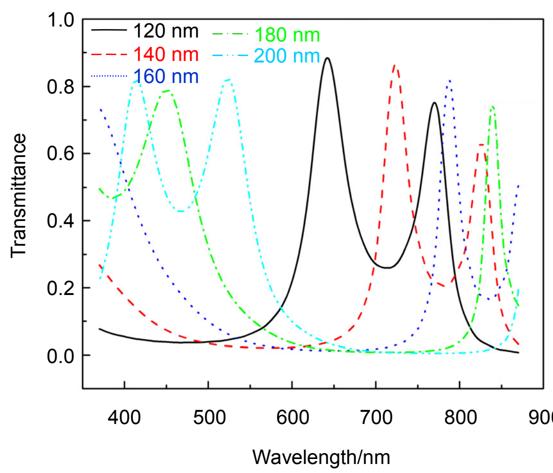

Fig. 5 Optical transmission spectra simulated using FDTD for normal incidence with 3.5 pairs of Ag/ITO layers consisting of 120 nm, 140 nm, 160 nm, 180 nm, and 200 nm ITO films, respectively, and a fixed Ag films thickness of 20 nm

Table 1　Characteristics of 1D-PBG with 3.5 pairs of Ag/ITO layers consisting of 120 nm, 140 nm, 160 nm, 180 nm, and 200 nm ITO films, respectively, and a fixed Ag films thickness of 20 nm

Sample structure (d_d, d_m, a, n)	Band gap range (λ_1~λ_2)/nm	Band gap (λ_2-λ_1)/nm	Central wavelength	$\Delta\lambda$/nm
(140,20,160,3.5)	427~628	201	527	-
(160,20,180,3.5)	496~755	259	625	98
(180,20,200,3.5)	551~815	264	683	58
(200,20,220,3.5)	597~863	266	726	43

decreasing. For instance, the red shift of the central wavelength $\Delta\lambda$ is 98 nm, 58 nm, and 43 nm, respectively, as each ITO layer thickness increasing with a step of 20 nm.

3.2 Reflection of Ag-PBG

In order to illustrate the effect of 1D M-D PBG structure on optical reflection, the reflection of samples with different thickness of ITO and Ag films were discussed. Each layer thickness of the ITO films was maintained at 60 nm, while the thickness of the Ag films ranged from 8 nm to 22 nm with a step of 1 nm. In Fig. 6, the wavelength range that corresponds to lower reflection (blue) becomes narrower as the Ag thickness increasing. Furthermore, reflection is enhanced for wavelengths above 750 nm, and the reflection region can be extend to 600 nm because the samples consisting of thicker Ag films have shorter plasmonic wavelengths and negative permittivity of higher absolute valie.

In contrast to Fig. 6, there are two low reflection areas ranging from 380 nm to 780 nm when the ITO thickness increases to 80 nm as shown in Fig. 7. As mentioned above, the two low reflection areas are induced by thicker ITO films. Besides, there is a reflective band in the longer and shorter wavelength areas of optical range, which is induced by a plasmonic stop band and a structure band, respectively. It is clearly seen that both of the reflective band broaden and increases after increasing the thickness of each layer Ag films.

The reflection at wavelength of human eye sensitivity (near 550 nm) is remarkably enhanced when the thickness of each layer ITO films increased to 120 nm as shown in Fig. 8. It similarly has two low reflection bands above 600 nm, but the both low reflective band significantly towards to longer wavelength with the decreasing of the thickness of Ag films. And the central wavelength of the two low reflection bands corresponds to 650 nm and near 750 nm respectively. According to Fig. 7 and Fig. 8, the same conclusion can be drawn: the distance between two low reflection bands decreases as the Ag thickness increasing. The plasmonic band gap is beyond to 780 nm. The reflection simultaneously increases, and the reflective band broadens accordingly at 550 nm. By-comparing Figs. 6~8, we found that the reflective band induced by the structure band gap red-shifts along with the unit size increasing and enhanced by increasing metal fraction. The reflective band owing to the plasmonic band gap as well as redshifts associated with metal fraction decreasing, and reflection enhanced by improve metal fraction. As mentioned above, the 1D M-D PBG not only improves optical transmittance but also enhances optical reflection, which is determined by both the unit size and the metal-thickness ratio.

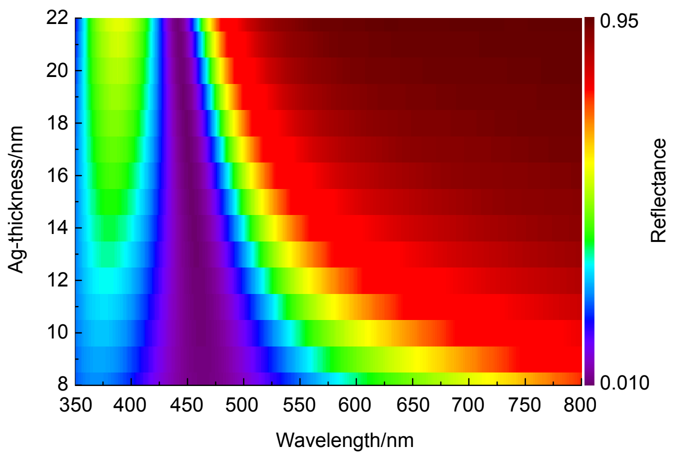

Fig. 6　Optical reflection spectra simulated using FDTD for normal incidence with 3.5 pairs of Ag/ITO, consisting of Ag with thicknesses from 8 nm to 22 nm, and a fixed ITO thickness of 60 nm

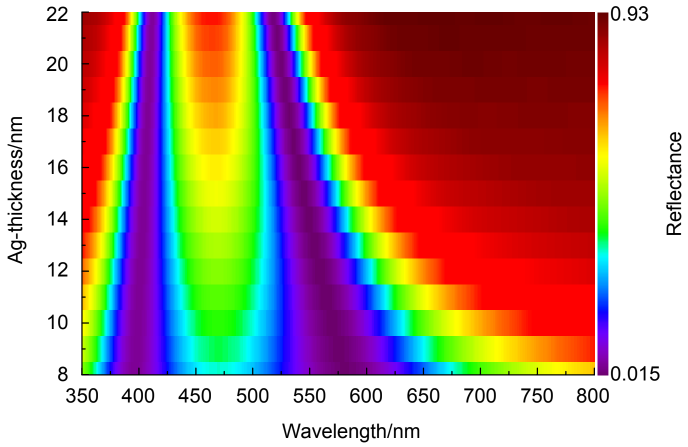

Fig. 7　Optical reflection spectra simulated using FDTD for normal incidence with 3.5 pairs of Ag/ITO with a Ag layer ranging from 8 nm to 22 nm thickness and fixed ITO thickness of 80 nm

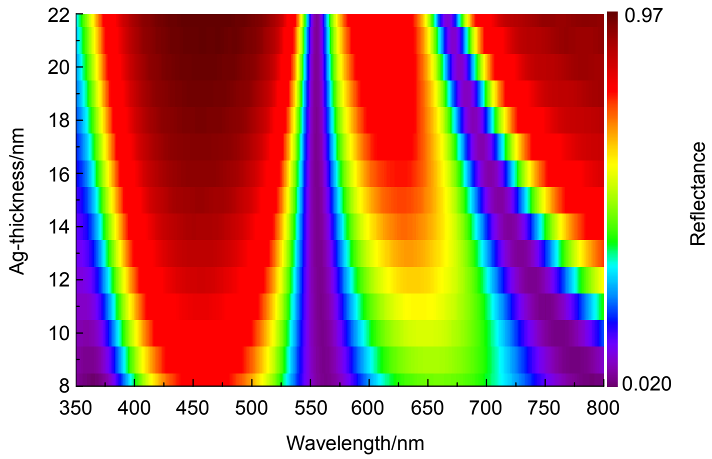

Fig. 8　Optical reflection spectra simulated using FDTD for normal incidence with 3.5 pairs of Ag/ITO with a Ag layer ranging from 8 nm to 22 nm and ITO films of 120 nm thickness

4　Conclusions

We have designed 1D M-D PBG using Ag and ITO layers with different thicknesses and studied their optical properties via FDTD. It is found that the incorporation of thicker dielectric layers can enhance optical transparency. When the thickness of ITO films included in 1D M-D PBG is below 60 nm, a peak appears in the transmission spectrum, and a minimum reflective band appears in the reflection spectrum. When each ITO layer is thicker than 60 nm, two transmission peaks and two reflective minima appear in the transmission and reflection spectra. In addition, the distance between the two reflective minima decreases as the ITO thickness increasing. When the unit size is below 80 nm, reflection for wavelengths that longer than the cutoff wavelength are larger and enhanced after increasing the thickness of the Ag films, Moreover, the cutoff wavelength shifts towards shorter wavelength accordingly. If the unit size is greater than 80 nm, a structure band gap and a plasmonic band gap simultaneously appear in the shorter and longer wavelength region of the optical spectrum. Moreover, the structure band gap shifts towards longer wavelength as the unit size increasing. Both the structure and plasmonic band gaps are broadened and deeper as the each thickness of Ag films becoming thicker. Once the each thickness of ITO films is 120 nm, there is a deeper structure band gap near the 450 nm. The reflection also enhance by improving the thickness of Ag films. As a result, both optical transmission and reflection can be adjusted by adopting appropriate structure. The results are very helpful for visual color design and optical filter production using 1D M-D PBGs.

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Optical characteristics of one dimensional metal-dielectric photonic band gap material

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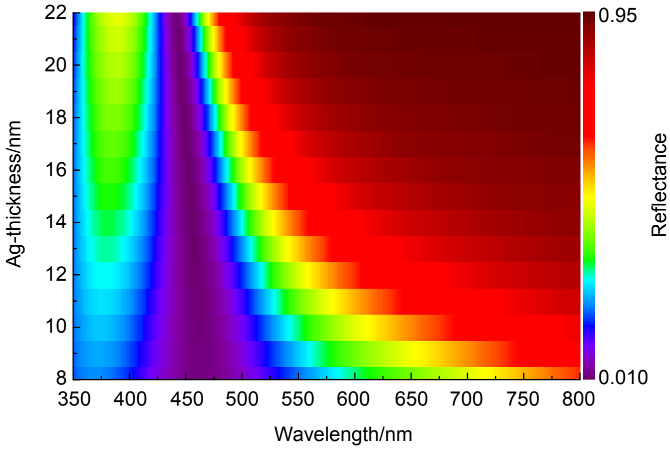

Optical reflection spectra simulated using FDTD for normal incidence with 3.5 pairs of Ag/ITO, consisting of Ag with thicknesses from 8 nm to 22 nm, and a fixed ITO thickness of 60 nm

Overview: This paper describes the optical transmittance and reflection of one dimensional metal-dielectric photonic-band gap material (1D M-D PBG), which is made of different thicknesses ITO and Ag layers. In this paper, there are two crucial factors determining optical transmittance were taken into account. One factor is that a structure band gap presents in the optical structure when the unit size is larger than 80 nm. The other factor is that the plasmonic band gap extends into the optical region with high metal fraction. The two factors have been never been discussed in past. The results are very helpful for visual color design and optical filter production using 1D M-D PBGs. The paper suggested that 1D M-D PBGs with lower than 100 nm ITO films favor to enhance their optical transmittance, and the structures with longer ITO films can induce improvement of optical reflection. In addition, both the reflection in structure and plasmonic band gap increases and broadens by increasing Ag films fraction. The reflection spectrum induced by structure and plasmonic shifts towards longer wavelength as a result of unit size and metal fraction increasing. It is found that the incorporation of thicker dielectric layers can enhance optical transparency when the ITO film thickness is lower than 80 nm. Once the thickness of ITO films included in 1D M-D PBG is below 60 nm, a peak appears in the transmission spectrum, and a minimum reflective band appears in the reflection spectrum. When each ITO layer is thicker than 60 nm, two transmission peaks and two reflective minima appear in the transmission and reflection spectra. In addition, the distance between the two reflective minima decreases as the ITO thickness increasing. Both the structure and plasmonic band gaps are broadened and deeper as the each thickness of Ag films becoming thicker. Once the each thickness of ITO films is 120 nm, there is a deeper structure band gap near the 450 nm. The reflection also enhance by improving the thickness of Ag films. As a result, both optical transmission and reflection can be adjusted by adopting appropriate structure. The results are very helpful for visual color design and optical filter production using 1D M-D PBGs.

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