Theoretical study on the photonic band gap in one-dimensional photonic crystals with graded multilayer structure*

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We theoretically investigate the photonic band gap in one-dimensional photonic crystals with a graded multilayer structure. The proposed structure constitutes an alternating composite layer (metallic nanoparticles embedded in TiO_2 film) and an air layer. Regarding the multilayer as a series of capacitance, effective optical properties are derived. The dispersion relation is obtained with the solution of the transfer matrix equation. With a graded structure in the composite layer, numerical results show that the position and width of the photonic band gap can be effectively modulated by varying the number of the graded composite layers, the volume fraction of nanoparticles and the external stimuli.

Keywords: graded photonic crystals, multilayer, band gap

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1. Introduction

Photonic crystals (PCs) are periodic arrays of materials with different refractive indexes, having the ability to control the flow of photons.[1–3] PCs have attracted wide research attention owing to their unique light-manipulation abilities, demonstrating wide applications in optical sensors, optical filters, and various optical integrated circuit devices.[4,5] To fabricate them, both top down (lithographic technique) and bottom up methods (nanoscale self-assembled method)[6] have been put forward to realize different structures like the slab,[7] the multilayer,[8] cylinder arrays,[9] or even the fractal structures.[10] Among them, one most studied structure is in the form of planar films,[11] where the periodic alternating layers are obtained by bottom-up assembly. This procedure is based on sequential spin-coating suspensions of nanoparticles on the substrates. With such a method, simple stable inexpensive PCs were obtained. Meanwhile, the modulation of the refractive index is achieved by alternating the size, type, and concentrations of nanoparticles in the composite layer or by controlling the number of deposited layers.[12,13] Moreover, PCs are able to be realized through a combination with channels, walls, or microfluidic chips,[14] where colloids are forced through the area with pressure. In most cases, the composite layer is a suspension of monodispersed colloids, composed of dielectric SiO_2 or TiO_2 particles.[12,15] However, if small metallic nanoparticles are introduced into a suspension, the third order Kerr-type nonlinearity of composites have to be included, resulting in an enhancement in the local electric field.[16,17] Simulation results have shown that tunable plasmon resonant effects arise with gold nanoparticles inserted into periodic PCs.[18]

In this paper, we theoretically study the dispersion relation in the graded multilayer structure through varying the number of deposited composite layers, the volume fraction of nanoparticles, and the external stimuli. The graded profile is along the direction perpendicular to the surface of the multilayer. Regarding the multilayer as a series of capacitance, the optical behavior in each layer is calculated. Numerical results about the photonic band position and band width are also presented. This work is organized as follows: In Section 2, we first illustrate the optical properties in the multilayer system, then introduce the transfer matrix method. This is followed by Section 3, in which numerically calculated results about dispersion relation in the proposed graded or linear multilayers are discussed. This paper ends with a conclusion in Section 4.

2. Formulism

PCs are artificial optical structures having a large refractive index contrast.[19] The major functionality of the photonic structure is the strong distortion or modification

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of dispersion, which can influence the behavior of photons. The realization of a photonic band gap depends strongly on its dimensionality.[20] Since a one-dimensional (1D) periodic structure has a degree of freedom only along its crystal axis. We focus on 1D graded PCs (GPCs) for simplicity. Graded materials are the ones whose material properties are spatially dependent. It has long been recognized that the gradients in layer composition can improve the performance of a material,[21] and open up the additional possibility of shaping the refractive contrast.[22–24]

Let us first consider a graded multilayer structure with N layers, the dielectric constant varies continuously along the z direction and in the i-th layer, the dielectric constant is expressed as $\varepsilon_{(i,z)}$. The schematic structure of our proposed 1D GPCs is illustrated in Fig. 1. It is composed of one composite layer and one air layer and the graded composite layer constitutes three layers with different nanoparticle volume fractions. For specificity, an Ag nanoparticle embedded in the TiO_2 is studied in the composite layer. For 1D PCs with an infinite period, the whole structure can be regarded as a series of multilayer structures, acting as an LC circuit. The reciprocal of the equivalent capacitance $C_{\rm eqv}$ of multiple capacitors connected in series is the sum of the reciprocals of the individual capacitances C_n. It can be expressed as $1/C_{\rm eqv} = 1/C_1 + 1/C_2 + ... + 1/C_n = \sum_{i=1}^{n}(1/C_n)$, where $C = \varepsilon s/4\pi k_{\rm c} d_s$, ε is the dielectric constant, s is the capacitor plates of area, d_s is the distance between capacitor plates, and $k_{\rm c}$ is the electrostatic constant. Thus, by using the equivalent capacitance of series combination, the optical response of the graded composite layer ε_1 can be expressed as

$$\frac{1}{\varepsilon_1} = \frac{1}{L}\int_0^L \frac{{\rm d}z}{\varepsilon_i(i,z)}, \tag{1}$$

where L is the thickness of the graded film, and it is divided into N layers. Due to the periodicity of two refractive index materials, the multilayer structure creates a periodic potential for photons in one dimension. Electromagnetic waves of a given frequency propagating through a stack of layers at normal incidence is considered.[25,26] Resorting to the solution of 1D Maxwell's equations, the electric and magnetic fields component along the incident light direction can be related via the transfer matrix. For 1D PCs with double layers, the dispersion relation is in the form as follows:

$$\begin{aligned}\cos(kd) &= \cos(k_1 a)\cos(k_2 b) \\ &\quad - \frac{1}{2}\left(\frac{k_1}{k_2} + \frac{k_2}{k_1}\right)\sin(k_1 d_1)\sin(k_2 d_2),\end{aligned} \tag{2}$$

where a and b are thicknesses of corresponding layers, d is the lattice constant and $d = a + b$, k represents the wave vector in the PCs, $k_1 = \omega\sqrt{\varepsilon_1}/c$ denotes the local wave vector of layer 1, and $k_2 = \omega\sqrt{\varepsilon_2}/c$ is the local wave vector of layer 2. Here, ω is the frequency of light or electromagnetic waves, and c is the speed of light in vacuum. The dielectric constant of air is taken as ε_0.

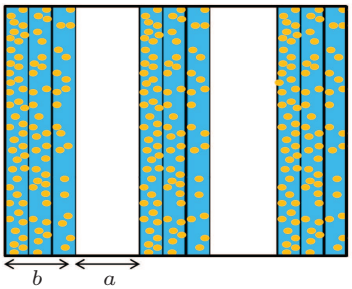


Fig. 1. (color online) Schematic structure of 1D GPCs is shown. It consists of the composite layer and the air layer. The width of the air layer and the composite are a and b respectively. In the composite layer, three layers with different volume fraction are illustrated.

As metallic nanoparticles are included in the composite film, the local electric field enhancement induced by the third-order nonlinearity has to be considered. With Ref. [16], the local electric field inside the nanoparticle can be written as $\varepsilon_1' = \varepsilon_{\rm Ag} + \varepsilon_k \chi^{(3)}$, where $\chi^{(3)}$ is the third-order nonlinearity, ε_k equals to $9|\varepsilon_{\rm TiO_2}|/|((2+p)\varepsilon_{\rm TiO_2} + (1-p)\varepsilon_{\rm Ag})|E_0$, and E_0 is the external electric field. The effective dielectric constant of the composite layer ($\varepsilon_{\rm e}$) can be given through the Maxwell–Garnett theory[17]

$$\frac{\varepsilon_{\rm e} - \varepsilon_{\rm TiO_2}}{\varepsilon_{\rm e} + 2\varepsilon_{\rm TiO_2}} = p\frac{\varepsilon_1' - \varepsilon_{\rm TiO_2}}{\varepsilon_1' + 2\varepsilon_{\rm TiO_2}}, \tag{3}$$

where p is the volume fraction of the nanoparticles in the composite suspension, $\varepsilon_{\rm TiO_2}$ is the dielectric constant of TiO_2 and fixed as $2.4\varepsilon_0$, and ε_1' is the dielectric constant of the nanoparticles and is taken as $-9.564\varepsilon_0$ for Ag nanoparticles, which is characterized by using the incident wavelength $\lambda = 497$ nm.[27]

3. Results and discussion

In this section, we present our numerical results (Figs. 2–7) of 1D GPCs consisting of the alternating air layer and Ag nanoparticle-based composite layer. With the incorporation of metallic nanoparticles, the local electric field induced by the external stimuli has to be included. Let x represent $\chi^{(3)}E_0$, the refraction index of the composite layers as a function of the external electric field stimuli x is illustrated in Fig. 2. It shows that the tunable refraction contrast can be obtained when x is changing from 0.0 to 1.0, indicating an enhanced magnitude of external field. With a different magnitude of the external field, the refraction index can effectively be tuned, and such spatial modulation opens up a forbidden gap in the electromagnetic dispersion relation.

Figure 3 shows the dispersion relations of the 1D GPCs with different numbers of composite layer N (2, 5, and 10). For the graded profile with 2 layers, $x = 0.1$, 0.6; 5 layers, $x = 0.1$, 0.3, 0.5, 0.7, 0.9; 10 layers, $x = 0.1$, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0. In each composite layer, the volume

fraction of the nanoparticles is fixed as $p = 0.15$. Equation 1 indicates that the composite layers with different numbers of layers will result in a change of the refraction index in each layer. From Fig. 3, we can clearly observe the photonic band gap moving towards the low frequency region when the number of layer N is closing to 10, and the photonic band width is getting wider with smaller $N = 2$. Thus, the band gap position and band gap width can effectively be tuned by changing N.

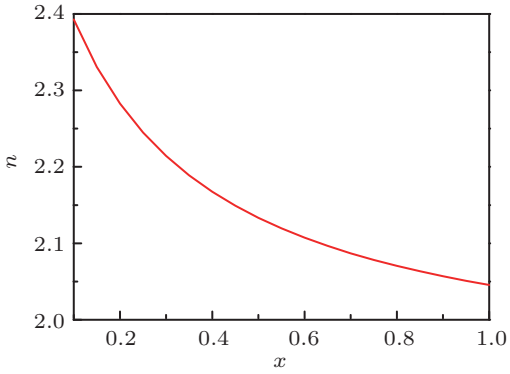


Fig. 2. (color online) Refraction index of the composite layer n as a function of the magnitude of the external electric field x is shown. Parameters: $p = 0.15$.

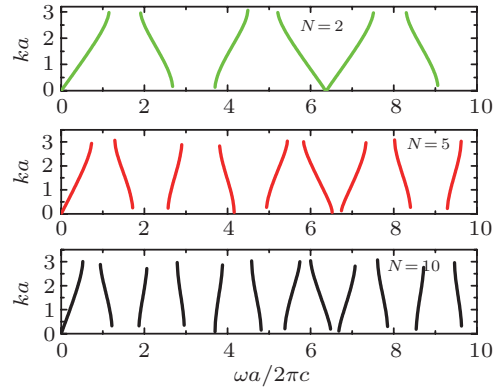


Fig. 3. (color online) The dispersion relation in graded multilayer structure with different N is illustrated, where the composite layer has 2, 5, 10 layers respectively. Parameters: $p = 0.15$. (From top to bottom: 2 layers, $x = 0.1$, 0.6; 5 layers, $x = 0.1$, 0.3, 0.5, 0.7, 0.9; 10 layers, $x = 0.1$, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0).

The results shown in Fig. 4 are for the same as Fig. 3, but in each composite layer, the volume fractions of the nanoparticles are different. For the graded profile with 2 layers, $p = 0.1$, 0.6; 5 layers, $p = 0.1$, 0.3, 0.5, 0.7, 0.9; 10 layers, $p = 0.1$, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0. With Eq. (3), our results show that the spectral position of the band gap can be effectively tuned by changing the volume fraction in each composite layer.

In Figs. 3 and 4, the graded profile (continuous variation in the magnitude of x or p) is investigated. Here, we focus on the linear profile, namely, the multilayer structure of PCs is purely composed of the air layer and composite layer with a fixed x or p. In Fig. 5(a), we can observe that the band gap position is moving towards the high frequency region with the increase of the magnitude of x. However, the band gap width is a constant even with different x as shown in Fig. 5(b), which is quite different from that of graded profile (Fig. 3). With a variation of volume fraction p in the composite layer, the results are shown in Fig. 6. In the low volume fraction, the photonic band gap position (Fig. 6(a)) moves towards the low frequency region. The first band width is also calculated in Fig. 6(b) in the green curve. It is found that the band width is still invariant in the linear profile even with different p.

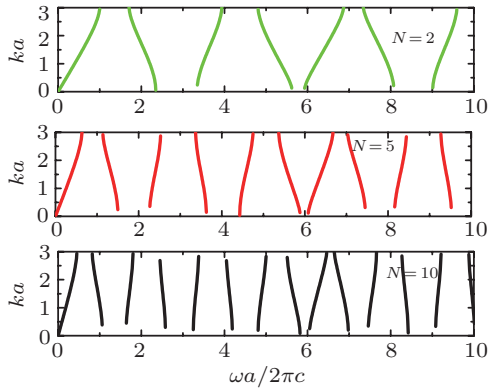


Fig. 4. (color online) The dispersion relation in graded multilayer structure with different p is illustrated, where the composite layer has 2, 5, 10 layers respectively. Parameters: $x = 0.1$. (From top to bottom: 2 layers, $p = 0.1$, 0.6; 5 layers, $p = 0.1$, 0.3, 0.5, 0.7, 0.9; 10 layers, $p = 0.1$, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0).

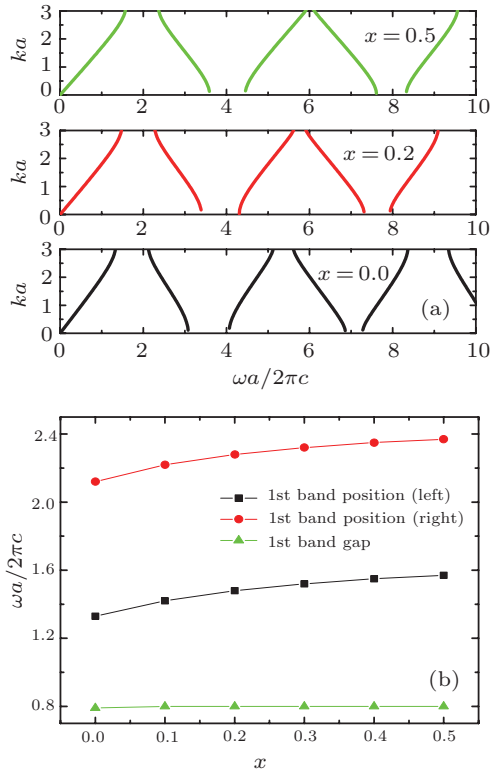


Fig. 5. (color online) (a) The dispersion relation in multilayer structure with different external stimuli ($x = 0.0$, $x = 0.2$, $x = 0.5$). (b) The position and width of the first band gap in the multilayer structure as a function of the applied field x. Parameters: $p = 0.15$, $a = 0.5$, $b = 0.5$.

In Fig. 7(a), we explore the dispersion relation with linear profile through the variations of the corresponding thicknesses of the two alternating layers. Here, we keep the lattice constant d as a constant. When the thickness of the composite

layer d_2 changes from 0.5, 0.7 to 0.9, the band gap position will move towards the high frequency region. Meanwhile, the first band gap width becomes larger with the increase of d_2, as shown in Fig. 7(b).

As we know, PCs are designed to affect the propagation properties of photons. The periodic spatial modulation opens up a forbidden gap in the electromagnetic dispersion relation. The wave propagation is affected when it enters into a material where some features (such as the topology, symmetry, refraction index contrast, etc.) are changed. In our proposed 1D GPCs, the refraction index can effectively be tuned by the external electric field, the volume fraction of the nanoparticles, and the number of graded composite layer. The modulation of the refraction index causes certain energies and directions to be forbidden for photons, which is called the photonic band gap. Resorting to the transfer matrix method, our results (Figs. 3–7) show that the position and width of the photonic band gap can effectively be modulated. With a proper structure parameter, the photonic band gap can be tuned to overlap with the electronic band edge, leading to the enhanced efficiency and the reduced noise in the operation of various optoelectronic devices. At the same time, the photonic band structure gives us information about the propagation properties of electromagnetic radiation within the photonic crystal.

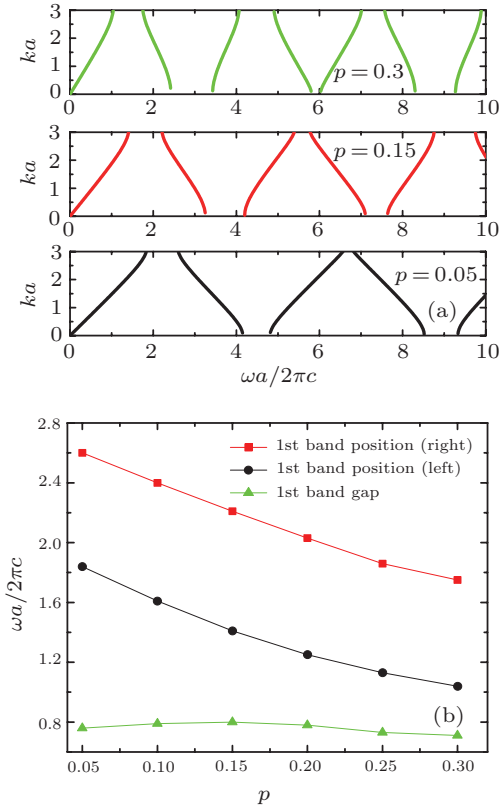


Fig. 6. (color online) (a) The dispersion relation in multilayer structure with different volume fraction of the nanoparticle ($p = 0.05$, $p = 0.15$, and $p = 0.3$). (b) The position and width of the first band gap in the multilayer structure as a function of the volume fraction p. Parameters: $x = 0.1$, $a = 0.5$, $b = 0.5$.

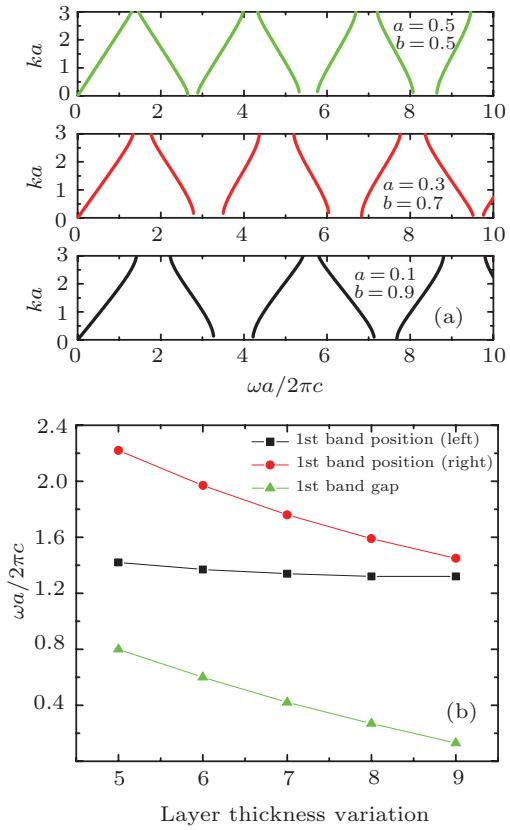


Fig. 7. (color online) (a) The dispersion relation in multilayer structures with different thicknesses in the composite layer. Parameters: $a = 0.5$, $b = 0.5$; $a = 0.3$, $b = 0.7$; $a = 0.1$, $b = 0.9$. (b) The position and width of the first band gap as a function of the thickness in the multilayer structure. Parameters: $x = 0.1$, $p = 0.15$.

4. Conclusion

In this work, we theoretically study the dispersion relation in 1D GPCs with a multilayer structure. For the composite layers, a silver nanoparticle embedded in the host medium is considered. Numerical results show that the tunable band gap and the band width can be realized with different numbers of composite layers, the volume fraction of nanoparticles. Moreover, the situation in the linear case illustrates that the photonic band moves to the high frequency region with a smaller p, a larger x or an increased thickness of the composite layer. Even with different p or x, the band gap width is invariant in the linear case. For such a graded structure, with fairly chosen structure parameters, a desired band gap and a band position can be obtained, which has the potential as an optical filter or works as a sensing material. Compared with the previous work, the tunability in our proposed structure is much easier to implement in the experiment (for example, the thickness of the composite layers can be increased with the additional spin coating process) with the guidance of our calculation results. Additionally, we want to mention that the photonic band gaps can also be tuned by different external stimuli such as magnetic fields,[28] temperature[29] or mechanical force.[30]

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