Optical Properties of a Periodic One-Dimensional Semiconductor-Organic Photonic Crystal*

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Abstract: Theoretical calculations via the transfer matrix method (TMM) are performed to investigate optical properties of one-dimensional semiconductor-organic photonic crystals (SOPC) with periodic conjugated polymer (3-octylthiophenes, P3OT)/AlN multilayer structure. The SOPC presents incomplete photonic band gap behavior in the UV region. P3OT/AlN multilayers with two pairs of 30nm-P3OT and 30nm-AlN layers exhibit a photonic band gap at a central wavelength of about 275nm, and the highest reflectivity reaches 98%. Furthermore, the band gaps are confirmed to be tunable by adjusting the lattice period and the filling fraction. As a consequence, the SOPC is important for achieving materials with an incomplete band gap in the UV region.

Key words: conjugated polymer; AlN; multilayer films; photonic band gap; TMM method
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1 Introduction

Recently, significant interest has arisen in artificial periodic dielectric structures with a period close to the wavelength of the electromagnetic (EM) wave[1~4]. Depending on the frequency requirement of specific applications, the engineering of structures that are periodic in 2D and 3D has been achieved for waves in the infrared, microwave, and millimeter wave region. For wavelengths shorter than infrared, only a few experimental and theoretical systems have been demonstrated to exhibit the signature of band gaps[5,6].

Organic materials have the advantages of flexibility, easier fabrication, and lower costs than inorganic materials. However, there are no reports on the optical properties of semiconductor-organic photonic crystals (SOPC). Conjugated polymers have been extensively studied as promising materials for applications in light-emitting diodes[7], displays[8], solar cells[9], and solid-state lasers[10]. One of the advantages of conjugated polymers is the simplicity of technological treatment due to the possibility of easy structural modification. Such materials demonstrate high nonlinearity and fast response[11], and have been used in fabricating photonic crystal structures in the visible range[12~14], such as polymer photonic crystal waveguides and conjugated polymer infiltrated in synthetic opal. In this paper, we report the optical properties of a one-dimensional SOPC with a periodic P3OT/AlN multilayer structure. Our calculated results suggest that absolute photonic bands of the SOPC can be tunable in the UV region by adjusting the structure of the SOPC. We believe that the properties of SOPCs offer potential applications in various photonic and electronic applications, especially in flexible or microcavity OLEDs.

2 Computational model and method

In our computational model, we consider a one-dimensional photonic band structure with different dielectric functions (ε_1, ε_2) and the same geo-material layer thickness (d_1, d_2). The 1D photonic crystal consists of an array of AlN and P3OT layers coupled to a homogeneous medium, characterized by ε_0 (such as the vacuum with $\varepsilon_0 = 1$) at the interface. The P3OT/AlN multilayers demonstrate the omnidirectional reflection over the wavelength range from 230 to 350nm. Electromagnetic waves are incident upon the multilayer films from the homogeneous medium. The generic system is illustrated in Fig. 1. The incident wave has a wave vector $\boldsymbol{k} = k_2\boldsymbol{i}_2 + k_3\boldsymbol{i}_3$ and a frequency $w = c|k|/\varepsilon_0$, where c is the speed of light in a vacuum and $\boldsymbol{i}_2$ and $\boldsymbol{i}_3$ are the unit vectors in the x and z directions, respectively. The wave vector together with the normal to the periodic structure defines a symme-

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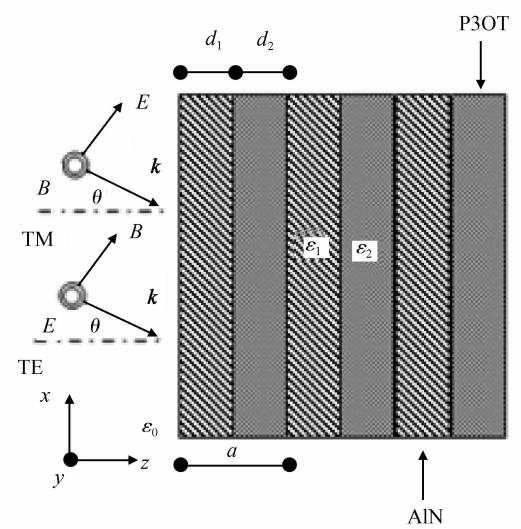

Fig. 1 Schematic of the multilayer system showing the layer parameters (ε_i and d_i are the dielectric function and thickness of layer i, respectively), the incident wave vector $\boldsymbol{k}$, and the electromagnetic mode convention E and B are the electric and magnetic fields, respectively.

try mirror plane that allows us to distinguish two independent electromagnetic modes: transverse electric (TE) and transverse magnetic (TM) modes. For TE/TM mode, the electric (magnetic) field is perpendicular to the plane. The propagation characteristics of an electromagnetic wave inside P3OT/AlN multilayers were calculated using the 'Translight' software package developed by the University of Glasgow[15,16]. This program is based on the transfer matrix method (TMM) and the original Photon program distributed by Pendry and his co-workers[15] at the Imperial College, London. The TMM method exploits Maxwell's equations by treating the full vector nature of the EM field when the wave-fields are expanded as an 'on-shell methodology'. This makes the calculations more efficient numerically and also allows calculating the reflection properties of photonic crystals. The calculation assumes that P3OT/AlN multilayers have finite thickness in the z-direction but are infinite in the x- and y-directions.

3 Results and discussion

We calculate reflectance spectra of P3OT/AlN multilayers for various thicknesses, assuming multilayers with an ideal structure. The dielectric functions of both P3OT and AlN are based on Kymakis and Benedict's optical data in UV[17,18]. The dielectric function is expressed as: $\varepsilon = \varepsilon' + i\varepsilon''$, The real and imaginary parts of the dielectric function, ε' and ε'' respectively, are determined for the P3OT and AlN layers. Figure 2 shows ε' and ε'' for P3OT and AlN. The H- and E-polarization reflectivity for a P3OT/AlN with a film thickness of about 60nm and the filling fraction d_1/a of 0.5 where d_1 is the thickness of the AlN layer and a is the thickness of layer pairs are shown in Figs. 3 (a) and 3(b). The spectra are taken for both H- and E-polarization with the $\boldsymbol{k}$ vector along the normal incidence direction (z axis). A PBG exists for H- and E-polarization ranges at wavelengths of around 275nm. An absolute photonic band gap is defined as the overlap region between the H- and E-polarization band

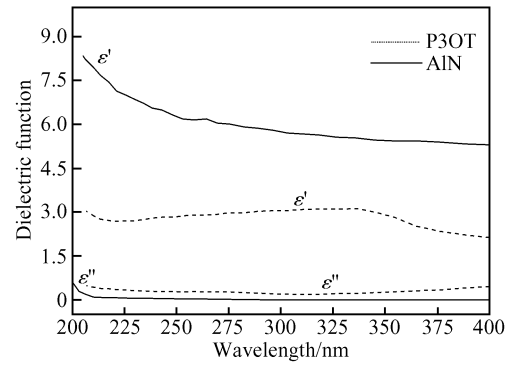

Fig. 2 Real and imaginary parts of the dielectric function of AlN and P3OT in UV region

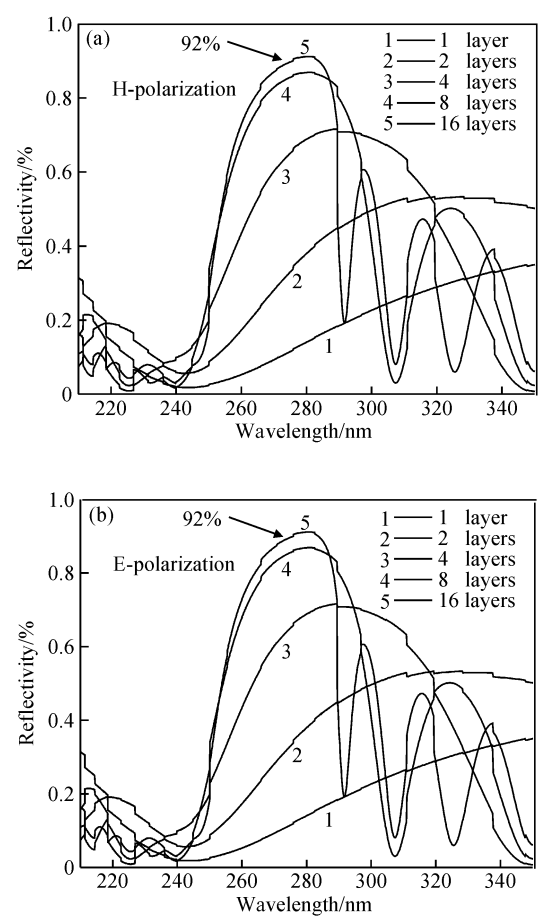

Fig. 3 Calculated reflectivities versus wavelength for H-polarization (a) and E-polarization (b) of P3OT/AlN multilayers

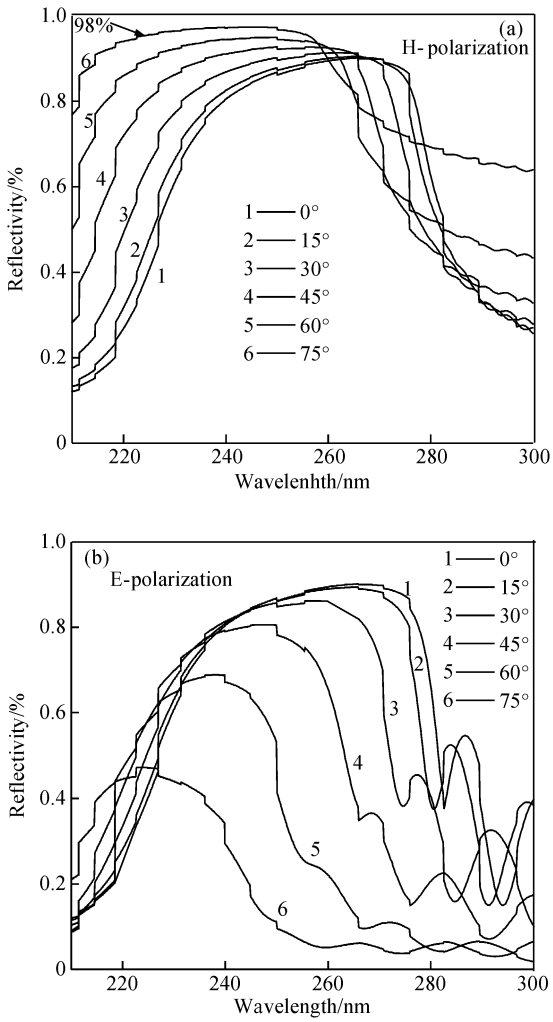

Fig. 4　Calculated reflectance spectra for P3OT/AlN multilayers for 0, 15, 30, 45, 60, and 75° incidence angles　(a) H-polarization; (b) E-polarization　Filling fraction (d_1/a) is 0.5, with 60nm thick layer pairs. The structure is 8 unit cells thick.

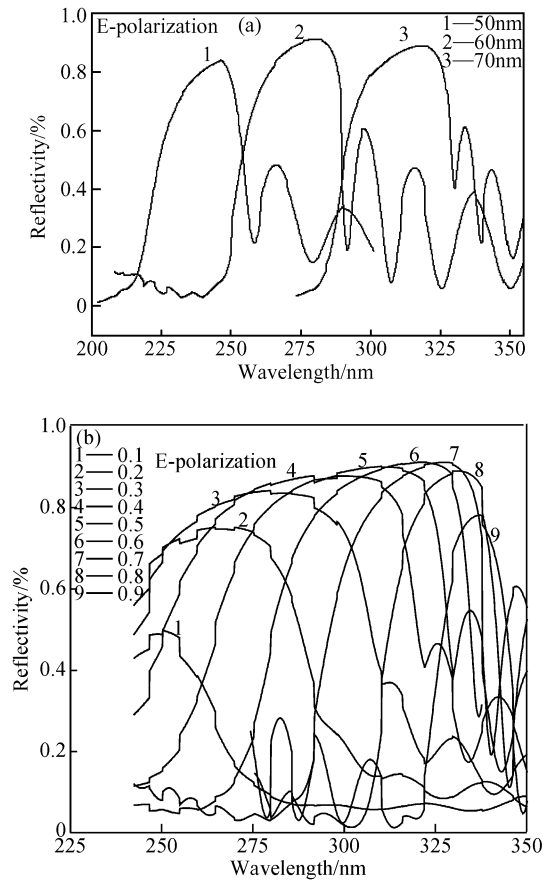

Fig. 5　Calculated reflection coefficients response for different lattice period (filling fraction $d_1/a = 0.5$) for E-polarization (a) and for different d_1/a (the lattice period $a = 70$ nm) for E-polarization (b)　The structure is 16 unit cells thick.

gap. Figures 3(a) and 3(b) show that their band gaps overlap. Meanwhile, reflectivity increases with the number of layer pairs, up to about eight pairs. Reflectivity almost saturates at around sixteen pairs, with a maximum of about 92%.

The dependence of the reflectance of the P3OT/AlN multilayer structure on the incidence angle is also investigated. The reflection spectra for H- and E-polarization modes is shown for a $\boldsymbol{k}$ vector (incident wave vector) lying in the xz-plane (off-plane propagation, meaning that the propagation is no longer along the z direction). In particular, a zero incidence angle corresponds to normal incidence where the $\boldsymbol{k}$ vector is parallel to the z axis.

The reflectance spectra for H-polarization are shown in Fig. 4(a). As the incidence angle increases, reflectivity increases. The maximum reflectance of the P3OT/AlN multilayers is 98% at 75° incidence for the H-polarization mode at a wavelength of about 250nm. The locality of the original band gap moves toward the lower wavelength region and the width of the original band gap changes, but not obviously, when $\boldsymbol{k}$ is in the x-z plane.

For E-polarization as shown in Fig. 4(b), as the angle of incidence increases, the locality of the original band gap moves toward the lower wavelength region and the width becomes narrow when $\boldsymbol{k}$ is in the x-z plane. However, the reflectivity decreases as the angle of incidence increases. This is due to increasingly compromised periodicity of the structure seen by the incident wave for tilted incidence. Figure 4 also shows that P3OT/AlN multilayer films are a PBG with an incomplete band gap.

We also calculated the reflection coefficients for the multilayer structures with different lattice periods (a) and filling fractions (d_1/a), and for normal incidence (k along the z-direction). The results are shown in Fig. 5. The results show that the width, depth, and the position of the PBG obviously change when using different values of a or d_1/a. As the lattice period changes from 50 to 70nm ($d_1/a = 0.5$), the band gap moves toward the higher wavelength region and the reflection coefficient has a maximum

value between 55 and 65nm. The peak reflection coefficient appears at around 60nm in Fig. 5(a). As the filling fraction changes from 0.1 to 0.9 (a = 70nm), the band gap moves toward the higher wavelength region, and the width of PBG has a maximum value at 0.5, as shown in Fig. 5(b). This suggests that we can perform fine-tuning on the band gap by changing the lattice period and the filling fraction.

4 Conclusion

Using the transfer matrix method we have calculated for the first time a one-dimensional semiconductor-organic photonic crystals (SOPC) in a P3OT/AlN multilayer structure with incomplete photonic bandgap for both E- and H-polarized radiation in the UV region. The SOPC with two pairs of 30nm P3OT and 30nm AlN layers exhibited a photonic band gap at a central wavelength of about 275nm and the highest reflectivity reached 98%. Moreover, the band gaps were confirmed to be tunable by adjusting the lattice period and the filling fraction. So the photonic crystal may be important for fabricating a photonic crystal with an incomplete band gap in the UV region.

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一维半导体-有机物型光子晶体的光学特性*

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摘要： 理论上采用转移矩阵法研究了具有 P3OT/AlN 多层膜结构的一维半导体-有机物型光子晶体的光学特性. 计算结果表明：由厚度分别为 30，30nm 的 P3OT，AlN 薄膜组成的多层膜结构，在中心波段为 275nm 处有一不完全的光子带隙存在，反射率最高可达 98%；而且可以通过调整薄膜厚度、填充比等参数对光子带隙的位置、反射强度进行调制. 因此，这种一维半导体-有机物型光子晶体对在紫外波段获得具有一定功能的光子晶体具有重要的指导意义.

关键词： 共轭聚合物；AlN；多层膜；光子带隙；转移矩阵法
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