# Optical properties in 1D photonic crystal structure using Si/$C_{60}$ multilayers*

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**Abstract:** The feasibility of using Si/$C_{60}$ multilayer films as one-dimensional (1D) photonic band gap crystals was investigated by theoretical calculations using a transfer matrix method (TMM). The response has been studied both within and out of the periodic plane of Si/$C_{60}$ multilayers. It is found that Si/$C_{60}$ multilayer films show incomplete photonic band gap (PBG) behavior in the visible frequency range. The fabricated Si/$C_{60}$ multilayers with two pairs of 70 nm $C_{60}$ and 30 nm Si layers exhibit a PBG at central wavelength of about 600 nm, and the highest reflectivity can reach 99%. As a consequence, this photonic crystal may be important for fabricating a photonic crystal with an incomplete band gap in the visible frequency range.

**Key words:** fullerene; Si; multilayer films; photonic band gap; TMM method
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## 1. Introduction

Recently, significant interest arises in the artificial periodic dielectric structures with a period close to the wavelength of 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 infrared, microwave, and millimeter wave regions. For wavelength shorter than infrared, only a few experimental and theoretical systems have recently been demonstrated to exhibit the signature of band gaps[5]. This is because most materials have high absorption coefficients and unstable dielectric constants under prolonged irradiation with UV/VIS light, together with difficulty in constructing samples with a small structure.

Many applications require the control of laser beams very close to plane waves. In this case, a 1D photonic crystal, e.g. dielectric multilayers is preferred. The 1D configuration can be easily fabricated by using existing techniques, and detailed investigations of the scattering process resulting in wave transmission become possible. The fullerenes are new and exciting materials[6–9]. High-quality $C_{60}$ thin films have been grown on various semiconductor and metal substrates, such as Si[10], Ge[11], GaAs[12], Ag[13], and Cu[14]. In recent years, much work has been done to investigate the interactions between $C_{60}$ overlayers and various semiconductor and metal surfaces. Up to now, most of previous works have been limited to the study of the structural and physical properties of fullerene multilayer films, there have been few investigations of the photonic properties of fabricating photonic crystal (PC) structures using the fullerene multilayer films.

In this paper, we study the possibility of using Si/$C_{60}$ multilayer films as one-dimensional photonic band gap crystals.

## 2. Computational model and method

In computational model, we consider a multilayer system where 1D PCs structures of materials Si and $C_{60}$ alternate. Si and $C_{60}$ are two dielectric materials, with different dielectric functions ($\varepsilon_1$, $\varepsilon_2$ ) and geo-material layer thicknesses ($d_1$, $d_2$), respectively. The 1D photonic crystal consists of an array of Si and $C_{60}$ layers coupled to a homogeneous medium, characterized by $\varepsilon_0$ (such as the vacuum with $\varepsilon_0 = 1$) at the interface. It needs to mention that $C_{60}$/Si multilayers demonstrate the omnidirectional reflection over the wavelength range from 390 to 750 nm. 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 $k = k_2 i_2 + k_3 i_3$ and a frequency $w = c|k| / \varepsilon_0$, where $c$ is the speed of light in vacuum and $i_2$ and $i_3$ are the unit vectors in the $x$ and $z$ directions, respectively. The wave vector together with the normal to the periodic structure defines a symmetry

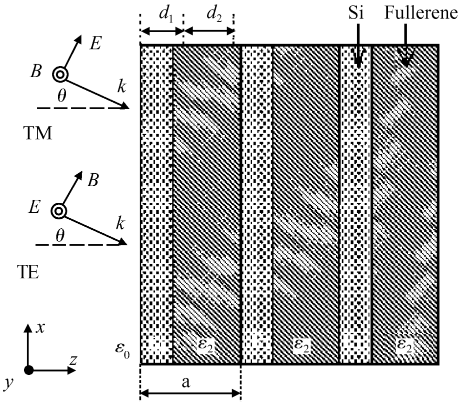

Fig. 1. Schematic of the multilayer system showing the layer parameters ($\varepsilon_i$ and $d_i$ are the dielectric function and thickness of layer $i$, respectively), the incident wave vector $k$, and the electromagnetic mode convention. $E$ and $B$ are the electric and magnetic fields, respectively.

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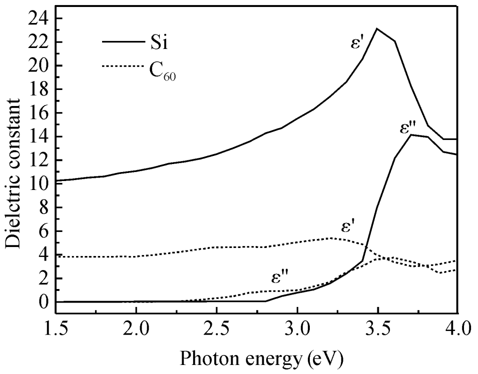

Fig. 2. Real and imaginary parts of the dielectric function of Si and $C_{60}$.

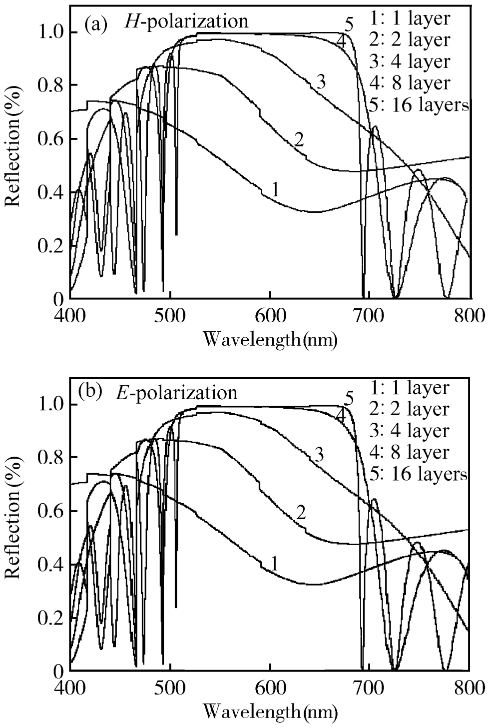

Fig. 3. Calculated reflectivities versus wavelength for (a) H-polarization and (b) E-polarization of $C_{60}$/Si multilayers.

mirror plane that can 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 Si/$C_{60}$ multilayers are calculated using a "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. 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 Si/$C_{60}$ multilayers have finite thickness in the $z$-direction but is infinite in the $x$- and $y$-directions.

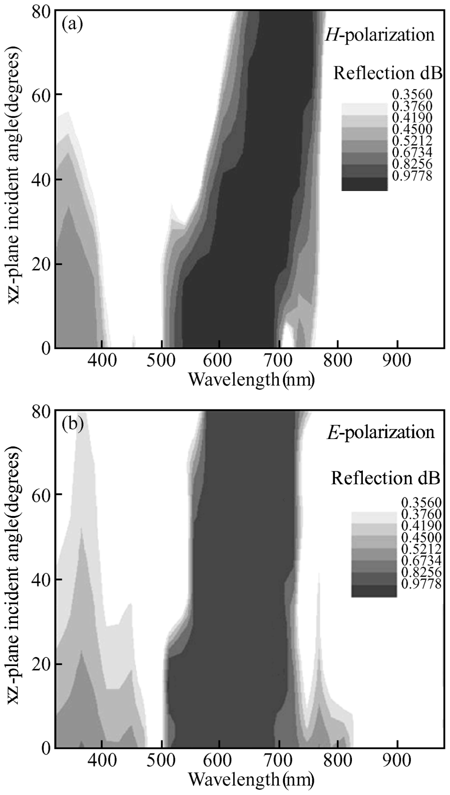

Fig. 4. Calculated in and out of plane angular response for $C_{60}$/Si multilayer structure, in which the zero angle of incidence corresponds to an incidence along the $z$-direction. Results for H-polarization are shown in (a) for an angular scan within the periodic $xz$-plane and (b) for E-polarization. Filling fraction ($d_1/a$) is 0.3, with thickness of layer pairs 100 nm. The structure is 16 unit cell thick.

## 3. Results and discussion

We calculate reflectance spectra of Si/$C_{60}$ multilayers for various thicknesses, assuming the multilayers with an ideal structure. The dielectric functions of both Si and $C_{60}$ are based on Palik and Kataura's optical data[17,18]. The dielectric function is expressed as: $\varepsilon = \varepsilon' + i\varepsilon''$, The real and imaginary parts of the dielectric function, $\varepsilon'$ and $\varepsilon''$ respectively, are determined for the Si and $C_{60}$ layers. Figure 2 shows $\varepsilon'$ and $\varepsilon''$ for $C_{60}$ and Si. The H- and E-polarization reflectivity for a Si/$C_{60}$ with a film thickness of about 100 nm and the filling fraction $d_1/a$ of 0.3 where $d_1$ is the thickness of the Si 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 $k$ vector along the normal incidence direction ($z$ axis). It can be seen that a PBG exists for H- and E-polarization ranging from 510 to 690 nm. An absolute photonic band gap is defined as overlap region between the H- and E-polarization band gap. Figures 3(a) and 3(b) show that their band gaps are overlapped. Meanwhile, reflectivity increases with the number of layer pairs, up to about eight pairs. Reflectivity almost saturates at around sixteen pairs, with the maximum of about 99%.

Figure 4 shows the reflection coefficients for a $k$ vector (incident wave vector) lying in $xz$-plane (off-plane propagation, meaning that the propagation is no longer along the $z$-direction). In particular, a zero angle of incidence corresponds to normal incidence where the $k$ vector is parallel to the $z$-axis. As the angle increases, the $k$ vector tilts toward the $x$-axis and the angle of incidence is measured between the $z$-axis and the $k$ vector. The reflection spectrum for H-polarization is shown in Fig. 4(a). As the angle of incidence increases, the locality of the original band gap moves toward higher wavelength region, and the width of the band gap is narrowed for $k$ lying in the $xz$-plane. For E-polarization as shown in Fig. 4(b), with increasing angle of incidence, the locality of the original band gap also moves toward higher wavelength region, and the width of the bandgap changes but not substantially for $k$ lying in the $xz$-plane. This is caused by the increasingly compromised periodicity of the structure seen by the incident wave for tilted incidence. Absolute band gap is seen to exist comparing Figs. 4(a) and 4(b). However, the gap width or the overlap region between the two polarization gaps decreases for increasing angle of incidence. The absolute PBG has a maximum value between 510–690 nm at 0°. Figure 4 also shows that Si/$C_{60}$ multilayer films are a PBG with an incomplete band gap.

## 4. Conclusion

Using the transfer matrix method, we have calculated a 1D photonic bandgap structure in the Si/$C_{60}$ multilayer films with absolute photonic bandgap for both E- and H-polarized radiation in the visible frequency range. The theoretical reflectance coefficients have been presented, the first to be calculated. A Si/$C_{60}$ multilayer with two pairs of 70 nm $C_{60}$ and 30 nm Si layers showed an incomplete PBG at central wavelength of about 600 nm, and this photonic crystal may be important for achieving materials with an incomplete band gap in the visible frequency range.

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## References

[1] Johnson S G, Fan S, Villeneuve P R, et al. Guided modes in photonic crystal slabs. Phys Rev B, 1999, 60: 5751

[2] Biswas R, Sigalas M M, Subramania G, et al. Photonic band gaps of porous solids. Phys Rev B, 2000, 61: 4549

[3] Jin C, Cheng B, Man B, et al. Two-dimensional dodecagonal and decagonal quasiperiodic photonic crystals in the microwave region. Phys Rev B, 2000, 61: 10762

[4] Notomi M, Tamamura T, Ohtera Y, et al. Direct visualisation of photonic band structure for three-dimensional photonic crystals. Phys Rev B, 2000, 61: 7165

[5] Xu Bingshe, Dang Suihu, Han Peide, et al. Band gaps of two-dimensional photonic crystal structure using conjugated polymer (3-octylthiophenes). Opt Commun, 2006, 267(2): 362

[6] Kasatani H, Terauchi H, Hamanaka Y, et al. X-ray-diffraction study of the phase transition in a $C_{60}$ single crystal. Phys Rev B, 1993, 47: 4022

[7] Moret R. Orientational ordering in the low-temperature phase of $C_{60}$ studied by single-crystal X-ray diffraction. Phys Rev B, 1993, 48: 17619

[8] Koma A. Van der Waals epitaxy—a new epitaxial growth method for a highly lattice-mismatched system. Thin Solid Films, 1992, 216: 72

[9] Xu H, Chen D M, Creager W N. Double domain solid $C_{60}$ on Si (111)-7 × 7. Phys Rev Lett, 1993, 70: 1850

[10] Hashizume T, Wang X D, Nishina Y, et al. Field ion-scanning tunneling microscopy study of $C_{60}$ on the Si (100) surface. Jpn J Appl Phys, 1992, 31: 880

[11] Xu H, Chen D M, Creager W N. $C_{60}$-induced reconstruction of the Ge (111) surface. Phys Rev B, 1994, 50: 8454

[12] Xue Q, Ling Y, Ogino T, et al. $C_{60}$ single crystal films on GaAs (001) surfaces. Thin Solid Films, 1996, 281: 618

[13] Giudice E, Magnano E, Rusponi S, et al. Morphology of $C_{60}$ thin films grown on Ag (001). Surf Sci Lett, 1998, 405: 561

[14] Motai K, Hashizume T, Shinohara H, et al. $C_{60}$ grown on the Cu (111) 1 × 1 surface. Jpn J Appl Phys, 1993, 32: 450

[15] Pendry J B, MacKinnon A. Calculation of photon dispersion relations. Phys Rev Lett, 1992, 69: 2772

[16] Bell P M, Pendry J B, Moreno L M, et al. A program for calculating photonic band structures and transmission coefficients of complex structures. Comput Phys Commun, 1995, 85: 306

[17] Palik E D. Handbook of optical constant of solids. London: Academic Press Inc Ltd, 1985: 350

[18] Kataura H, Endo Y, Achiba Y, et al. Dielectric constants of $C_{60}$ and $C_{70}$ thin films. J Phys Chem Solids, 1997, 58: 1913