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One–dimensional TiO$_2$/SiO$_2$ photonic crystal filter for thermophotovoltaic applications

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Abstract

Background: The efficiency of a thermal conversion system requires adequate radiative properties. In a thermophotovoltaic system, the optical filter plays a key role into the overall performance of the system. The purpose of this paper is to study a one-dimensional TiO$_2$/SiO$_2$ photonic crystal for application as thermophotovoltaic optical filter.

Methods: The influence of the layers' thicknesses, incidence angle, and number of periods on the spectral reflectance has been investigated through the transfer matrix method.

Results: It was found that, when one varies the number of layers from 6 to 12, an improvement of the optical properties of the spectral filter is observed. The surface wave through a film of photonic crystal generates a resonant transmission for a truncated structure.

Conclusions: These results are in conformity with those found in the literature.

Keywords: Thermophotovoltaic, Spectral filter, Transfer matrix method, Photonic crystal, Multilayered structures

Background

Thermophotovoltaics (TPVs) convert thermal radiation from a man-made high temperature source into electricity through photovoltaic (PV) cells [1, 2]. The concept dates back to 1960s [3]. A TPV system consists of a thermal radiator, PV cells, and selective filter. Low band-gap III–IV semiconductors have led to high performance of modern TPV systems. Advantages of TPV include high power density, good reliability, fuel versatility, low maintenance, and possibility of cogeneration (electricity and heat).

As the temperature of the radiator is typically in the range of 1200–1800 K, the fraction of the power above the electronic band-gap (Eg) in the total radiated power is quite small even for GaSb cells (with a low band-gap of 0.7 eV), leading to an extremely poor overall system efficiency and power density. Fortunately, the system performance can be significantly improved using a selective filter, which reflects below band-gap photons back to the radiator for re-radiation and transmits above band-gap photons to the cells. One dimensional (1D) Si/SiO$_2$ photonic crystals (PhCs) [4–6] were reported to be promising candidates for these kind of filters.

Most of the investigations on TPV systems focus on increasing conversion's efficiency and power density. For such purpose, the spectral control of thermal radiation from an emitter to a photovoltaic cell is important. One of the effective approaches for the spectral control is to use a filter that control photons selectively from an emitter to a photovoltaic cell. The filter in a TPV system plays its role in the following two aspects: (1) recycling thermal radiation, i.e. reflecting photons whose wavelengths are above the band gap wavelength of a photovoltaic cell back to the emitter. This action helps to maintain a high temperature level of the emitter and reduce the cooling load of the photovoltaic cell. (2) transmitting photons selectively, i.e. selecting the photons from an emitter whose wavelengths are below the band gap wavelength of a photovoltaic cell to

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penetrate the filter and reach the cell. These photons can be absorbed and stimulate electrons out of the photovoltaic cell. The need to develop suitable filter stimulated investigation to improve the conversion's efficiency of TPV systems. Several research groups have been devoting their work to filter's performance, and typical filter structures have been proposed including plasma filters [7, 8], one-dimensional Photonic Crystal [4, 9] filter, and frequency selective surface [6, 10].

One dimensional-photonic crystals (1D-PhCs) were used as selective filters in TPV systems. They present the advantages of being structurally simple and easy to be manufactured. A cascaded inhomogeneous dielectric substrate with different refractive indexes was designed as a frequency-selective structure (FSS), and used as selective filter for TPV system [11]. A 1D photonic crystals consisting of a dielectric-dielectric multilayer (Si/SiO$_2$) mounted on the top part of a TPV cell was used in both thermophotovoltaic (TPV) and micro thermophotovoltaic (MTPV) systems. They presented high efficiency and power throughput [12]. 1D metallic-dielectric photonic crystals (1D-MDPCs) of (Ag/SiO$_2$) were also designed [5] and studied [3]. O'Sullivan et al. [4] proposed and designed a 10-layer quarter-wave periodic structure (Si/SiO2) with thicknesses of 170 and 390 nm and suggested to reduce the first layer thickness to one half of its original thickness for better performances. In this paper, the use of TiO$_2$/SiO$_2$ (1D-PhCs) as selective filter for TPV systems with GaSb PV cell is proposed and studied using the transfer matrix method.

Methods

The assessment of the electric and magnetic fields in a periodic multilayered structure include several calculations' techniques. Banerjee et al. [13], successfully used Transfer Matrix Method (TMM) to evaluate the electric and magnetic fields in a metamaterial structure consisting of positive index materials (PIM) and negative index materials (NIM) alternating structure in both TE and TM modes. The results were compared to those using standard finite element methods (FEM). It was found that the TMM calculations are less computationally demanding, not limited by the thickness of the structures and can be performed for arbitrary angular plane wave spectra. The TMM approach can also be readily applied to a wide variety of cases, such as beam propagation through induced reflection gratings in nonlinear media.

Presentation of the transfer matrix method

The transfer matrix method (TMM) is widely used for the description of the properties of stacked layers [14, 15]. It provides an analytical means for calculation of wave propagation in multilayered media. The method

permits exact and efficient evaluation of electromagnetic fields in layered media through multiplications of 2×2 matrices. The solution of the coupled modes (TE and TM) equations is represented by a 2×2 transfer matrix which relates the forward and backward propagating field amplitudes. The grating structure is divided into a number of uniform grating sections, each with its own analytic transfer matrix. The transfer matrix of the entire structure is obtained by multiplying the individual transfer matrices together [16]. The boundary conditions for the vectors of the electric field E in each side of an unspecified interface allow a simple description by a 2×2 matrix. For the kth interface, the relationship between the components of the field is given by [13]:

$$\begin{pmatrix} E_{k-1}^+ \\ E_{k-1}^- \end{pmatrix} = D_{k-1,k} \begin{pmatrix} E_k'+ \\ E_k'- \end{pmatrix}, \tag{1}$$

where

$$D_{k-1,k} = \frac{1}{t_{k-1,k}} \begin{pmatrix} 1 & r_{k-1,k} \\ r_{k-1,k} & 1 \end{pmatrix}, \tag{2}$$

The field components at the left and right sides of the kth layer are defined by the propagation matrix P_k [13]:

$$\begin{pmatrix} E_{k^+} \\ E_{k^-} \end{pmatrix} = p_k \begin{pmatrix} E_k^+ \\ E_k^- \end{pmatrix}, \tag{3}$$

where

$$P_k = \begin{pmatrix} \exp(i.\phi_k) & 0 \\ 0 & \exp(-i.\phi_k) \end{pmatrix}, \tag{4}$$

$\phi_k = \frac{2.\pi.n_k \cos(\theta_k)}{\lambda}.d_k$ represents the dephasing for $\theta \neq 0$
The transfer matrix of the system is:

$$M_k = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} = D_k.P_k.D_{k, k+1}, \tag{5}$$

For N layers, the transfer matrix is given by the following relation [13]:

$$M = M_1.M_2 ....M_N, \tag{6}$$

One can directly determine the coefficients of transmission and reflection as [13]:

$$r = \frac{M_{21}}{M_{11}} \text{ and } t = \frac{1}{M_{11}}, \tag{7}$$

Fresnel's coefficients are written [13]:

- For a parallel polarization (S):

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$$r_k^s = \frac{E_{k-1,r}^s}{E_{k-1,i}^s} \text{ and } t_k^s = \frac{E_{k,i}^s}{E_{k-1,i}^s}, \tag{8}$$

- For a perpendicular polarization (P):

$$r_k^p = \frac{E_{k-1,r}^p}{E_{k-1,i}^p} \text{ and } t_k^p = \frac{E_{k,i}^p}{E_{k-1,i}^p}, \tag{9}$$

These coefficients are expressed as functions of the refractive indexes n_{k-1} and n_k of the layers using Fresnel laws as follows [13]:

$$r_k^s = \frac{n_{k-1}\cos(\theta_k) - n_k\cos(\theta_{k-1})}{n_{k-1}\cos(\theta_k) + n_k\cos(\theta_{k-1})} \quad t_k^s = \frac{2n_{k-1}\cos(\theta_{k-1})}{n_{k-1}\cos(\theta_k) + n_k\cos(\theta_{k-1})}, \tag{10}$$

$$r_k^p = \frac{n_{k-1}\cos(\theta_{k-1}) - n_k\cos(\theta_k)}{n_{k-1}\cos(\theta_{k-1}) + n_k\cos(\theta_k)} \quad t_k^p = \frac{2n_{k-1}\cos(\theta_{k-1})}{n_{k-1}\cos(\theta_{k-1}) + n_k\cos(\theta_k)}, \tag{11}$$

In case of normal incidence ($\theta_k = 0$), the values of the Fresnel coefficients are independent to the polarization condition. We therefore have:

$$r_k^s = r_k^p = \frac{n_{k-1} - n_k}{n_{k-1} - n_k}, \tag{12}$$

$$t_k^s = t_k^p = \frac{2}{n_{k-1} - n_k}, \tag{13}$$

For θ = 0, the dephasing is:

$$\phi_k = \frac{2.\pi.n_k}{\lambda}.d_k, \tag{14}$$

The energy conservation equation gives [13]:

$$|r|^2 + |t|^2 = 1, \tag{15}$$

$$R = |r|^2 \text{ and } T = |t|^2, \tag{16}$$

Modeling and evaluation of the system

In this paper, we study a TPV system with a spectral filter emitting light toward a GaSb cell. A 1D-PhCs is deposited on NaCl substrate which also serves as front encapsulation glass to a GaSb cell, separated from the emitter by 1 cm. Transfer matrix method is used to assess the performance of the system through the evaluation of the spectral efficiency. We used GaSb as PV cell, which has a low-direct band gap energy of 0.7 eV, corresponding to a wavelength of 1.78 μm. The performance of the 1D-PhCs TiO_2/SiO_2 filter is characterized by spectral efficiency which can be defined as the ratio of the above-band gap power transmitted through the filter to the PV cell to the net power of the filter got from the emitter [4]. In this paper we will show that the use of a 1D-PhCs TiO_2/SiO_2 structure as a selective filter can provide better spectral efficiency and system performance.

Spectral distribution of the thermal transmitter

Thermophotovoltaic (TPV) cells convert thermal radiation emitted from a thermal source directly into electricity (Fig. 1). The thermal transmitter behaves like a black body. It entirely absorbs radiations received from the heat source. To improve the reflectance and the spectral transmittance of the one-dimensional filter, the structure (TiO_2/SiO_2 PhC) must correspond to the spectral distribution of the transmitter at high temperature in the corresponding band of the reflectance and transmittance [7, 16]. According to Planck's law, the spectral power of the radiation of the source at high temperature is [7]:

$$E_{(\lambda,T)} = \frac{2\pi hc^2}{\lambda^5\left(\exp\left(\frac{hc}{\lambda KT}\right) - 1\right)}, \tag{17}$$

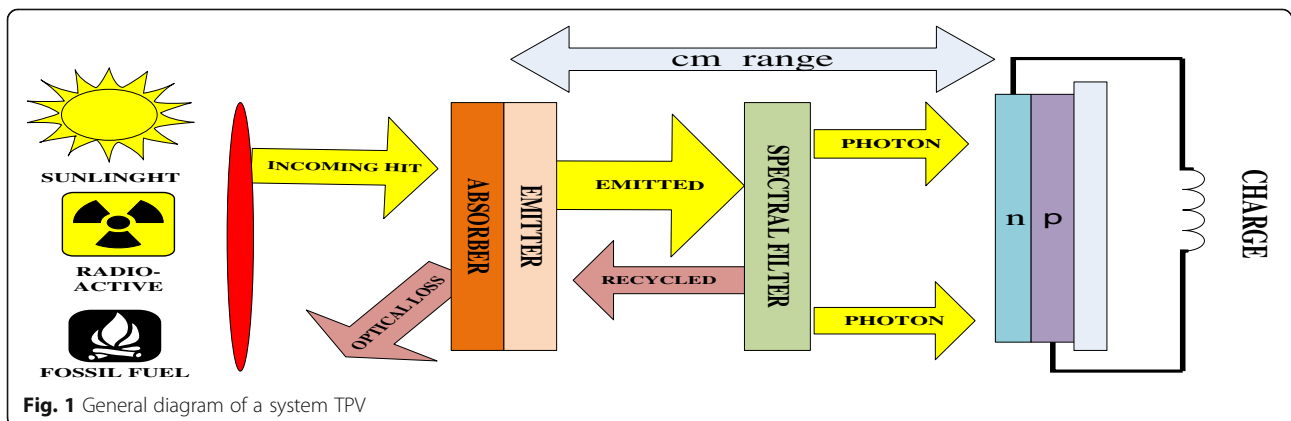where h is the Planck's constant, K the Boltzmann constant and c the speed of the light in the vacuum.

Fig. 1 General diagram of a system TPV

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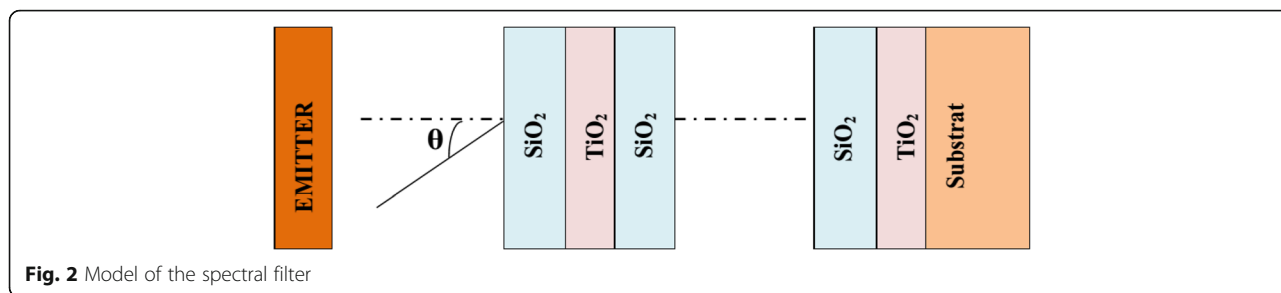
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Fig. 2 Model of the spectral filter

The total power radiated by a body is given by Stefan's law [7]:

$$P = \sigma T^4 \tag{18}$$

The wavelength (λ_m) of the maximum of radiated energy depends on the temperature T following the expression known as Wien's displacement law [7]:

$$\lambda_m . T = 2898 \ \mu m . K, \tag{19}$$

Studied model

We propose a structure made up of one-dimensional photonic crystals $(TiO_2/SiO_2)^6$ with P periods of Titanium Dioxide (TiO_2) and Silicon Dioxide (SiO_2) deposited on a substrate (NaCl). 1D-PhCs does not exhibit a complete photonic band gap. However, when coupled to free space it exhibits total omnidirectional reflectance, which can be used in TPV systems to improve its performance [17–19].

The central wavelength of the normal-incidence stop-band can be expressed as [19]:

$$\lambda_0 = \frac{1}{1 - \frac{2}{\pi} \sin^{-1}\left(\frac{n_H - n_L}{n_H + n_L}\right)} \lambda_g, \tag{20}$$

$$d_k = \frac{\lambda_0}{4 n_k}, \tag{21}$$

For thermal energy transformation into electric power, the photovoltaic cell which operates perfectly in the infrared is GaSb. Its energy of gap is Eg = 0.7 eV and its wavelength of gap is λg = 1.78 μm. The TiO_2 and SiO_2 used for the filter are respectively high (H) and low (L) refractive index materials. The refractive indexes are n_H = 2.4 for TiO_2 and n_L =1.46 for SiO_2. The substrate material for the filter has a refractive index taken as n_b = 1.5 in the entire range of wavelengths. The central wavelengths are located in the spectral band around 1300 nm. Figure 2 presents the model of the studied structure.

Results and discussion

The parameters that play an important role in achieving the best performance of the filter are the number of periods P, the thickness of each TiO_2 and SiO_2 layer, and the incidence angle.
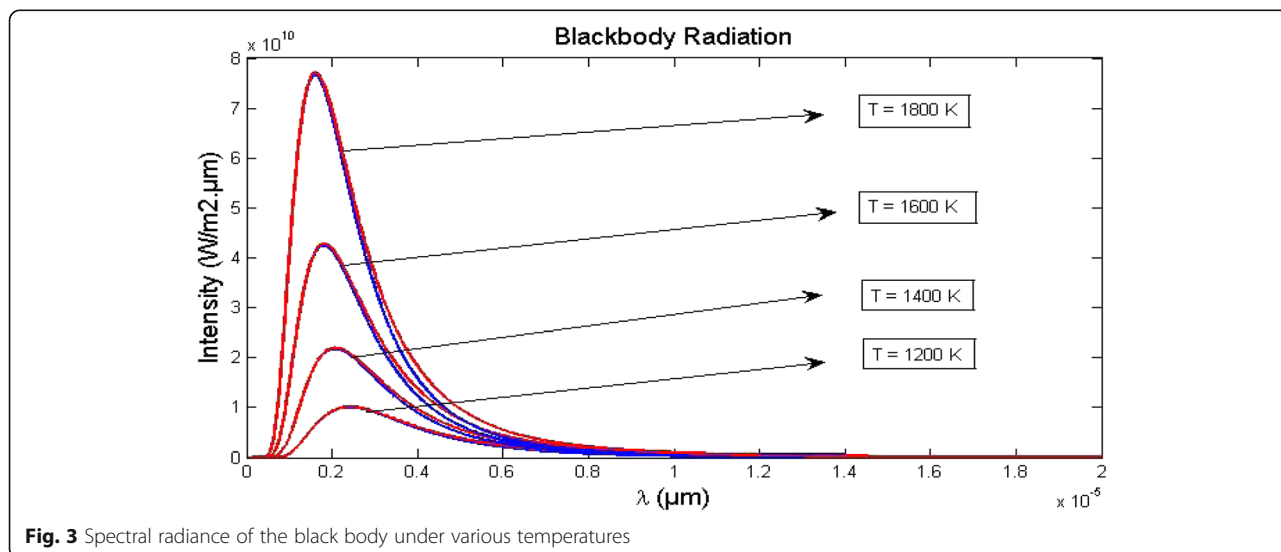

Fig. 3 Spectral radiance of the black body under various temperatures

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Behavior of the temperature of the transmitter

One of the important issues for improving the spectral transmission performance of the one-dimensional TiO_2/SiO_2 PhCs filter is to make the filter structure match well with spectral distribution of high temperature emitter within the corresponding transmission band. For the sake of analysis simplicity, the emitter is set as a blackbody [7, 16, 20]. The results corresponding to the wavelength range below 2000 nm are given in Fig. 3. It could be seen that, most of the radiation power from an emitter was limited in the spectral range of 0–2000 nm. Thus, the design of the filter should ensure this wavelength band to be in its high transmission band. Figure 3 presents an overview of the amount of light available for the GaSb cell. The red lines in the figure indicate the fraction of photons from the spectrum that is greater than the energy band gap.
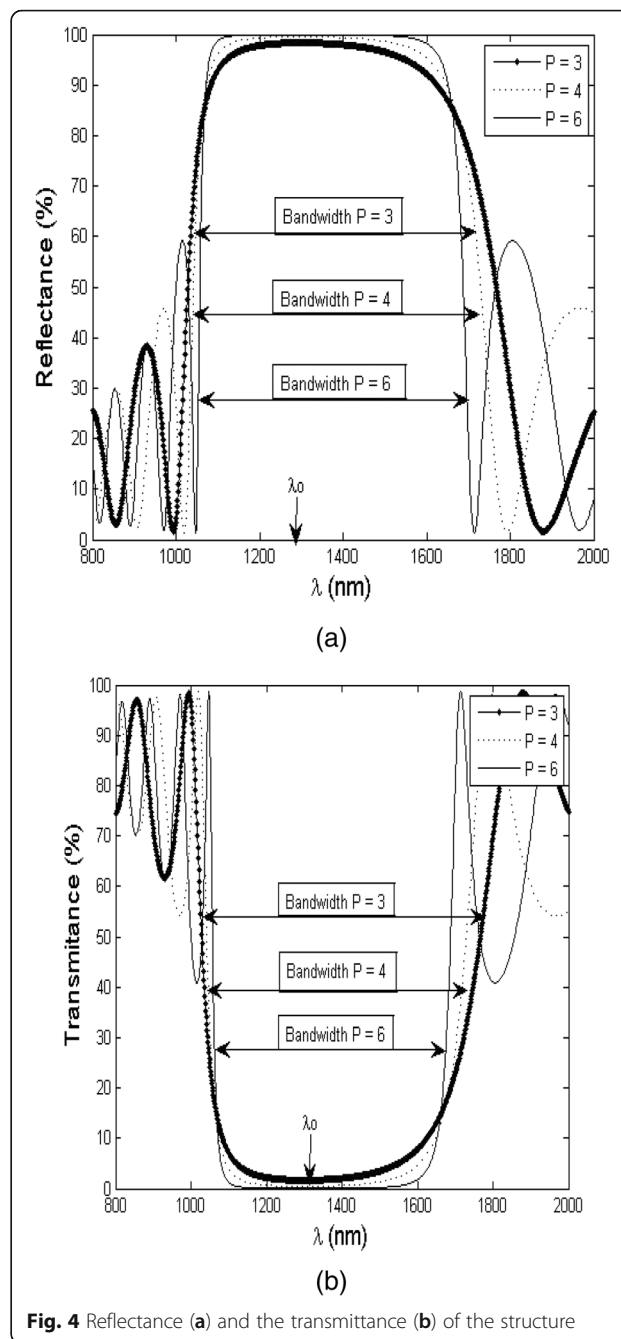
Effect of the number of periods on the reflectance and transmittance

Table 1 presents the values of the transmission and the reflection when the period varies.

The reflectance and transmittance of the structure are obtained by the TMM polarized in TM mode. Figure 4 shows the behavior of the multilayered structure at different periods. In Fig. 4(a), the reflection becomes flatter in the bandwidth $\Delta\lambda$ and reaches 100% when the number of period P increases from $P = 3$ to $P = 6$. In Fig. 4(b), the transmittance rapidly vanishes on bandwidth $\Delta\lambda$ when the period $P = 6$. These results are in conformity with those obtained by Li et al. [21, 22]. In fact, when the wave is generated inside the periodically nonlinear photonic crystal, its spatial evolution inside the 1D-PhCs is coupled to the spatial distribution. However, the structure encounters significant multiple reflections and transmission caused by the variation of the refractive index. Therefore, large oscillations appear in the pass band due to mismatch between the PhCs and the quartz substrate and these oscillations will lead to reduce the amount of power transmitted to GaSb cell. A large enhancement of the conversion efficiency can be obtained by the use of a one-dimensional photonic band gap structure such as a Bragg mirror, where the enhancement comes from the simultaneous availability of a high density of states. The combination of the quasi-phase matching and the photonic band edge effects in a nonlinear
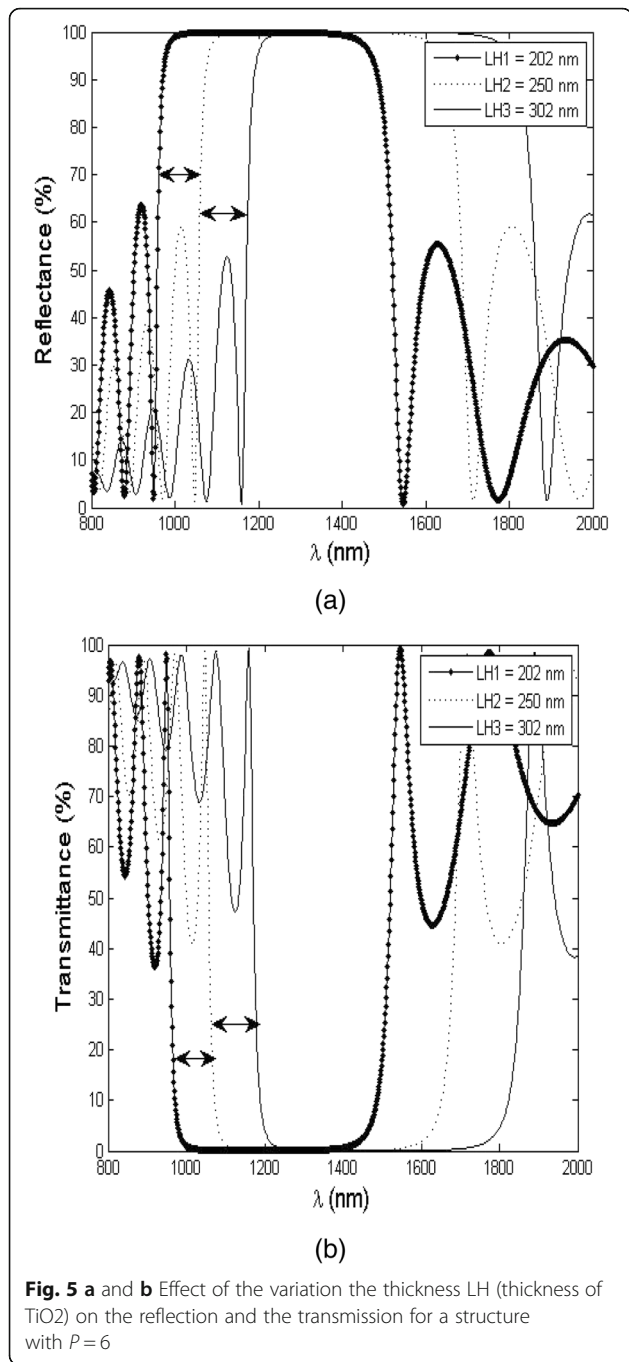

Fig. 4 Reflectance (**a**) and the transmittance (**b**) of the structure

structure with periodically poled crystals can significantly increase conversion efficiency, often three-four orders of magnitude compared to using quasi-phase matching only. The period of a nonlinear structure enables substantially to increase the conversion efficiency [21, 22].

Effect of the thickness of the layers on the reflectance and transmittance

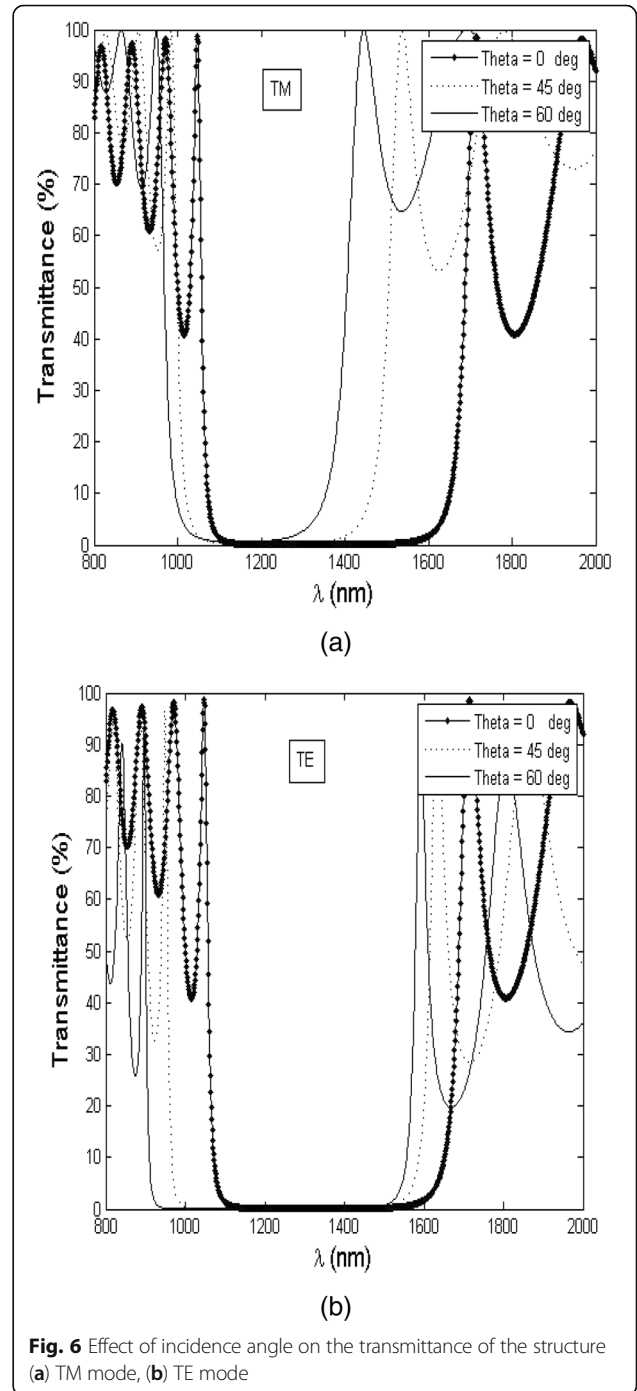Figure 5 presents the reflectance and transmittance of a 1D (TiO2/SiO2) photonic crystal deposited on a sodium

Table 1 Values of the reflection and the transmission when P varies

	λ_1 (nm)	λ_2 (nm)	$\Delta\lambda$ (nm)
$P = 3$	1160	1570	410
$P = 4$	1180	1150	270
$P = 6$	1200	1400	200

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Table 2 Value of the reflection and the transmission when LH varies

LH (nm)	λ_1 (nm)	λ_2 (nm)	$\Delta\lambda$ (nm)
202 nm	1000	1400	400
250 nm	1100	1480	380
302 nm	1220	1700	480

Fig. 5 a and **b** Effect of the variation the thickness LH (thickness of TiO2) on the reflection and the transmission for a structure with $P = 6$

chloride substrate (NaCl) for TM polarization. Table 2 shows the values of the transmission and the reflection when the thickness varies.

Effect of the incidence angle on the transmittance

The transmittance of the proposed structure for TM and TE modes is shown in Fig. 6. Table 3 presents the effect of incidence angle on the transmittance of the structure for both TM and TE modes.

Fig. 6 Effect of incidence angle on the transmittance of the structure (**a**) TM mode, (**b**) TE mode

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Table 3 Values of the bandwidth when the angle of incidence varies

	TM			TE		
	λ_1 (nm)	λ_2 (nm)	λ_1 (nm)	λ_2 (nm)	λ_1 (nm)	λ_2 (nm)
Theta = 0 degree	1100	1480	380	1100	1480	380
Theta = 45 degree	1090	1400	310	1000	1580	580
Theta = 60 degree	1080	1250	170	950	1500	550
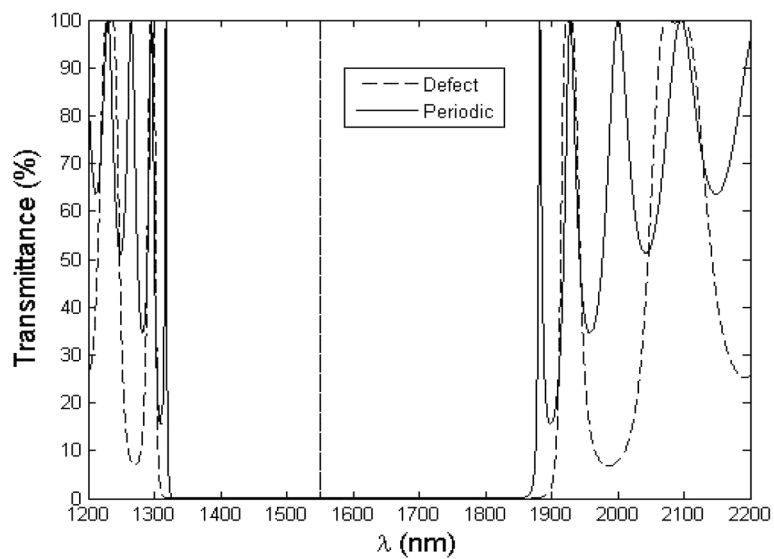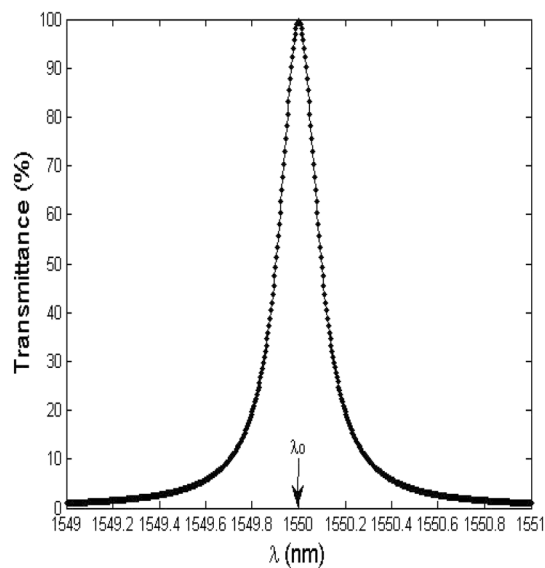
Fig. 7 a Transmission spectrum of the defect structure at incidence normal polarization TM. **b** Represents of the peak of transmission of the defect layer

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When the wave is polarized at normal incidence, both TE and TM modes present similar band gap. However, when the angle of incidence increases to 45°, there is a difference between the TE and the TM modes. The forbidden band becomes narrower when the incidence angle of the light is 60°; the TE polarization transmission spectrum moves rapidly to smaller wavelengths, while in the TM polarization, the movement is gradual. It could also be seen that when the incidence angle increases, the spectral transmittance decreases in passband region. Local field enhancement in a 1D-PhCs structure by introducing an oblique incidence angles may be larger than normal incidence. Oblique incidence provides a simple technique to tune the phase matching and local field enhancements for the sample. It is shown that widely different conversion efficiencies can be obtained for various incidence angles and various thicknesses of the nonlinear material [21, 23]. However, the variation of the angle of incidence allows obtaining different values of the efficiencies of the device; this is in line with the results obtained by Li et al. [22]. They calculated the spatial distributions of the fundamental frequency (FF) and second harmonic (SH) waves. Furthermore, they showed that widely different conversion efficiencies can be obtained for various incident angles of the FF of the nonlinear material.

Transmission through truncated film
The transmission spectrum is obtained when the film is illuminated by a monochromatic wave at normal incidence. The calculation is done in TM polarization as presented in Fig. 7. The considered wavelength range is between 1100 and 2200 nm. The designed wavelength at which the layers are quarter wavelength is taken to be the standard source λo = 1550 nm. Figure 7(a) presents the factor of transmission depending of the length of the wave in the case of truncation and no truncation. A peak of transmission of 100% appears in the gap about 1550 nm in the case of truncated photonic crystal. Figure 7(b) shows the resonance peak corresponding to the transmission of the truncated structure. The resonance at the transmission is provided by the excitation of surface waves at the interface of the film of the photonic crystal.

Conclusion
In this paper, we studied a one-dimensional TiO_2/SiO_2 photonic crystal as a spectrally selective filter for TPV applications. The transfer matrix method was used and the influence of the radiative properties (reflectance and transmittance) of the structure was assessed. The processor used in our work is an AMD Dual Core E-450 APU 1.65 GHz with 4 GB of memory for 12-layer structure. The solutions obtained by this method showed that for a 12-layer structure, the solution takes about 1.1 s; this is in

line with the results in obtained by Banerjee et al. [13]. The variation of period and layer's optical thicknesses LH permitted to evaluate the behavior of the structure. The effect of the angle of incidence on the spectral transmittance was also studied in both TM and TE polarization modes. It was found that, a suitable choice of wavelength's value in a well-defined range could lead to 100% resonant transmission.

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