One –Dimensional Si/SiO_2 Photonic Crystals Filter for Thermophotovoltaic Applications

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Abstract: - In this paper, a one - dimensional Si/SiO_2 photonic crystals (1D-PhCs) is optimized for potential application as thermophotovoltaic (TPV) optical filter. The performance of the proposed structure, 1D eight-layer Si/SiO_2 of thermophotovoltaic system, is studied. The effect of the thickness of layers, incidence angle and number of periods on the spectral reflectance has been investigated by rigorous coupled-wave analysis (RCWA) method. Both the original proposed and the modified structures were prepared through a magnetron sputtering technique. The measured results are in good agreement with the simulated results. The spectral efficiency value of the modified structure is 33.5%at emitter temperature of about 1500 K .The measured results and simulated results have shown that the modification introduced in the 1D Si/SiO_2 PhC has significantly improved the system performance.

Key-Words: - Filter, Photonic crystals, Reflectance Rigorous coupled wave analysis (RCWA), Thermophotovoltaic.

1 Introduction

Thermophotovoltaic (TPV) systems are capable of converting thermal infrared radiation directly into electricity by using photovoltaic effect. They have been considered as energy conversion systems, which allow recycling of the waste heat as well as increasing the conversion efficiency [1-3]. The TPV system consists of heat source and an optical cavity which comprises as a thermal radiator (emitter), a selective filter and a photovoltaic PV cell. TPV system promises to be a very clean, efficient, quiet, portable, reliability and a safe source of electrical power. As a result, TPV system can be used in transportation and aerospace power applications. It has a very good potential to be an alternative to traditional batteries [1-7]. The most obvious drawbacks of TPV devices are their low throughput and poor conversion efficiency, due to the absence of suitable emitters for the TPV cells [8].

The emitter temperature in a TPV system generally ranges between 1000 and 2000 K. It is suitable for PV cells with energy gap between 0.5 and 0.75 eV [3, 9-11]. Photons having energies higher than the TPV cell bandgap would be absorbed within the depletion region and could produce electricity. Photons having energies less than the TPV cell bandgap (sub-band gap photons) would be absorbed beyond the depletion region due to the long penetration depth of the material at these wavelengths, and cannot produce electricity. These sub-bandgap photons will result in a destructive heat load on the system components, which will lower the conversion efficiency of the system. In order to reduce the heating and to improve the TPV overall efficiency, these photons should be sent back to the emitter by using filter and back surface reflectors [1, 10]. GaSb, which has low- direct band gap energy of 0.7 eV, is optimum for an emitter temperature of about 1600 K, corresponding to a wavelength of 1.78 µm. This makes it a good choice for a TPV system which transfers the photon energy into electricity. An ideal filter should have low reflectance at short wavelengths and high reflectance at long wavelengths, compared to the bandgap energy [3, 10, 12]. A highly efficient TPV device demands the optimization of the output power and throughput. For such purpose, the spectral control of thermal radiation using a selective filter is playing an important role.

One dimensional-photonic crystals (1D PhCs) were used as selective filters in TPV system. They have the advantage of simple structure and that they can easily be fabricated. A cascaded inhomogeneous dielectric substrate with different refractive indexes was tailored as a frequency-selective structure (FSS) and was used as a selective filter for TPV system [13]. 1D photonic crystals which consists of dielectric - dielectric multilayer (Si/SiO_2) mounted on top of a TPV cell were used in both thermophotovoltaic TPV and micro thermophotovoltaic MTPV systems. They exhibited high efficiency and high power throughput [14]. 1D metallic - dielectric photonic crystals (1D MDPCs) which consists of (Ag/SiO_2) were fabricated [15] and theoretically studied [3]. O'Sullivan et al. [16] proposed and fabricated a 10-layers quarter-wave periodic structure (Si/SiO_2) with the thickness 170 and 390 nm, respectively and suggested reducing the first layer thickness to one half of its original thickness. Mao et al. [11] proposed and fabricated a 1D ten layers by using Si/SiO2 PhC. In this paper, the use of 1D Si/SiO_2 (1DPhCs) as selective filter for TPV system having GaSb PV cell is proposed and numerically studied.

2 Calculation Method

Rigorous coupled-wave analysis (RCWA), formulated in the 1980s by Moharam and Gaylord, is used for analyzing the diffraction of electromagnetic waves by periodic gratings [17]. It is used in this study to simulate the radiative properties (spectral emittance) of the periodically, micro-structured surfaces. It analyzes the diffraction problem by solving Maxwell's equations accurately in each of the three regions (input, multilayer, and output), based on Fourier expansion [18]. In RCWA, diffraction efficiency for each diffraction order is calculated with incident wave properties regardless of feature size, structural profiles, and dielectric function of the materials. The dielectric function of the materials is expressed as $\varepsilon = (n+ik)^2$, where n is the refractive index and k is the extinction coefficient. The accuracy of the solution computed depends solely upon the number of terms retained in space harmonic expansion of electromagnetic fields, which corresponds to the diffraction order.

3 Thermophotovoltaic System Modeling

In this paper we analyzed a TPV system that consists of a blackbody (BB) emitter separated from a GaSb cell array. A 1D PhC is deposited on quartz substrate which also serves as the front encapsulation glass of a GaSb cell and this is separated from the emitter by a few centimetres as shown in Fig.1. RCWA method [18] is applied to evaluate the performance of the TPV system by calculate the spectral efficiency. We use GaSb cell as PV cell, which has a low- direct band gap energy of 0.7 eV, corresponding to a wavelength of 1.78 µm and with refractive index n = 3.9. The performance of the 1D Si/SiO_2 PhC filter is characterized by spectral efficiency which can be defined as the ratio of the above-bandgap power transmitted through the filter to the PV cell to the net power the filter got from the BB emitter[16] can expressed as

$$\eta_{sp} = \frac{\int_{E_g}^{\infty} \frac{2\pi E^3}{c^2h^3} \frac{1}{\exp(E/kT_{emt}-1)} \varepsilon_{emt}(E) \bar{T}_f(E) dE}{\int_0^{\infty} \frac{2\pi E^3}{c^2h^3} \frac{1}{\exp(E/kT_{emt}-1)} \varepsilon_{emt}(E)\left(1-\bar{R}_f(E)\right) dE} \qquad (1)$$

Where $\bar{T}_f$ is the average transmittance of the filter (including both TE and TM transmittances), $\bar{R}_f$ the average transmittance of the filter and $\varepsilon_{emt}(E)$ is the hemispherical emittance of the emitter. Therefore

$$\bar{T}_f(E) = \int_0^{\theta_m} \left(T_{fTE}(E,\theta) + T_{fTM}(E,\theta)\right)\cos\theta\sin\theta d\theta \qquad (2)$$

$$\bar{R}_f(E) = \int_0^{\theta_m} \left(R_{fTE}(E,\theta) + R_{fTM}(E,\theta)\right)\cos\theta\sin\theta d\theta \qquad (3)$$

TE and TM are the two types of polarization (electric and magnetic modes respectively) and θ is the angle of incidence of radiation and $\theta_m = \pi/2$. The electromagnetic wave is incident from air at an incidence angle θ is assumed to be linearly polarized.

An ideal filter should have high transmittance for above bandgap photons $\left(T_{13}=1 \text{for} E>E_g\right)$ and low transmittance for low bandgap photons $\left(T_{13}=0 \text{for} E<E_g\right)$ back to the emitter. In this paper will show that the use of a 1D Si/SiO_2 structure as a selective filter can provide enviable spectral efficiency and system performance.

4 Proposed Structure

The proposed structure consists of one dimensional photonic crystals $(Si/SiO_2)^4$ deposited on a quartz substrate. A 1D PhC does not exhibit a complete photonic bandgap however, when coupled to free space it does exhibits total omni-directional reflectance, which can be utilized in TPV systems to improve system performance [19-20]. The central wavelength of the normal-incidence stop-band can be expressed as:

$$\lambda_0=\frac{1}{2}\left(1+\frac{2+\frac{4}{\pi}\sin^{-1}\frac{n_{Si}-n_{SiO2}}{n_{Si}+n_{SiO2}}}{2-\frac{4}{\pi}\sin^{-1}\frac{n_{Si}-n_{SiO2}}{n_{Si}+n_{SiO2}}}\right)\lambda_g \qquad (4)$$

Where λ_g is the normal incidence bandgap edge (1.78 μm for GaSb cell), n_{Si}=3.4 and n_{SiO2}=1.5 are the refractive indices of Si and SiO_2respectively. The layer thicknesses for Si and SiO_2 were use 170nm and 420 nm respectively.

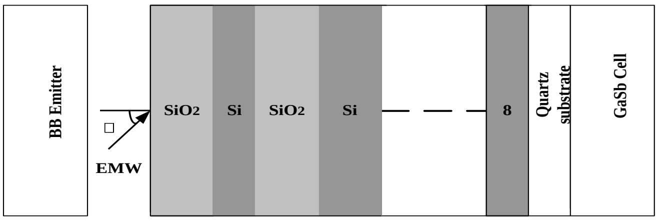


Fig.1 TPV system with a front side dielectric stack filter (1D PhC) deposited on quartz substrate on a GaSb cell that extends to + ∞

5 Fabrication of 1D Photonic Crystal

The original proposed structure an eight layer Si/SiO_2 1D PhCs which is detailed in previous section were prepared through a magnetron sputtering process. A mid-frequency reactive magnetron sputtering system (JGP450, Shenyang Co. Ltd.) was used to deposit the designed PhCs. The sputtering power was kept at 150W to obtain a desired layer and the base vacuum level was 6.2×10^{-4}Pa .The sputter targets were done in an argon Ar gas with the flow rate 30 SCCM and controlled by a mass flowmeter and the sputtering pressure about 1.9 Pa. The deposition process was carried out firstly before the PhC fabrication. A single Si target layer was deposited on quartz substrate for 900 s and a single SiO_2 target layer was deposited on crystalline silicon substrate for 3600 s. The layer thickness was obtained by an ellipsometer. The thickness for all sputtering targets after deposited on to substrates per unit of time can measure by using these equations

Si: $y = 5.9215x$ (5)

SiO_2: $y = 211.7887x$ (6)

Where, y the thickness of layer per (nm) and x time of deposition per minute, in equation (6) time per hours. A scanning electron microscopy (SEM) was used to study the surface morphology of the fabricated structures. The SEM used was a Helios Nanolab -600i. Fig.2 shows SEM image of the fabricated proposed structure cross section.

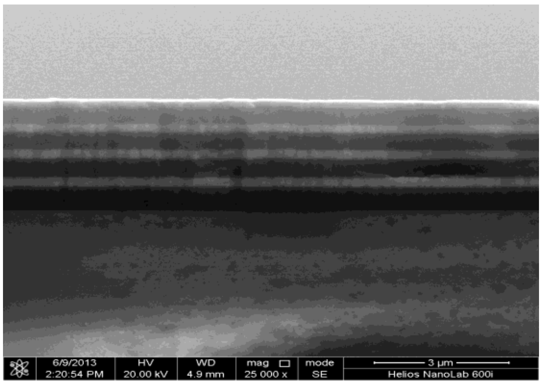


Fig .2 SEM image of the cross section of proposed structure before half of the top layer (SiO_2) was etched away

6 Results and Discussion

6.1 Effect of the Thickness of Layers on the Reflectance

The parameters that play an important role to achieve the best performance of the filter are the number of periods, P, the thickness of each Si, and the thickness of each SiO_2 layer. The TPV system consists of a blackbody emitter (BB) at temperature 1500 K, a selective filter and a GaSb photovoltaic cell. The normal incidence reflectance of 1D $(Si/SiO_2)^4$ PhC deposited on a quartz substrate for TM wave exhibits a wide stop-band as shown in Fig.3 (a). Large oscillations appear in the pass band due to mismatch between the PhC and the quartz substrate and these oscillations will lead to reduce the amount of power transmitted to GaSb cell. The original proposed structure has highest reflectance value exceeds 0.4 for radiated photons at $\lambda < 1.73\mu m$. However it reflects most of the radiated photons at $1.73\mu m < \lambda < 3.9\mu m$ utilizing the main high reflectance region based on the stop-band.

In order to reduce the pass band reflectance and improve the performance of the filter we need to reduce the first layer of SiO_2 to half of its original thickness to form anti-reflection coating. Fig.3 (b) shows the normal reflectance of the modified structure for TM wave. It has low reflectance in pass-band compared with the original structure. To evaluate the performance of the original proposed structure and modified structure we simulated the spectral efficiency as a function of the BB emitter temperature. Fig.4 shows the dependence of the spectral efficiency on the emitter temperature for both structures of the filter. The value of the spectral efficiency is about 0.335 for the modified structure at 1500 K emitter temperature, while it is only 0.300 for the original proposed 1D PhC filter. The normal transmittance for the original proposed and modified structure shown in Fig.5.

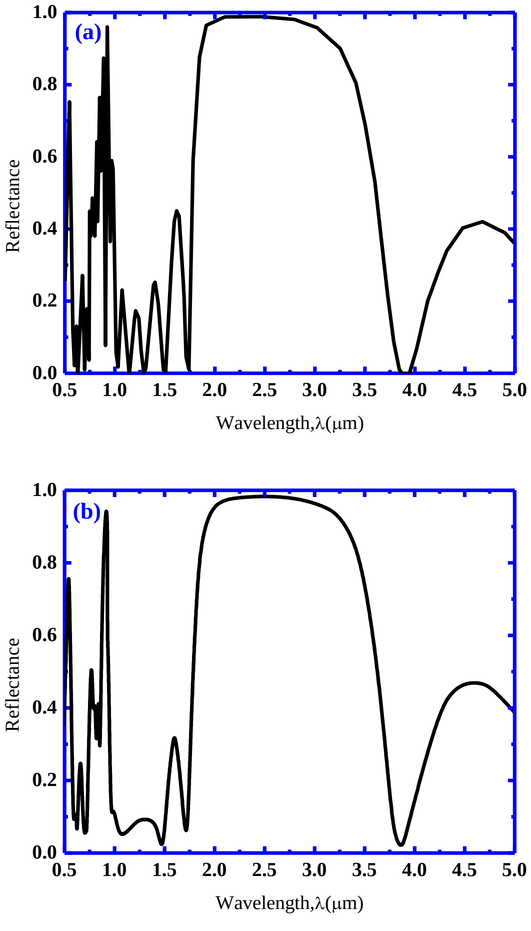


Fig.3 (a) Normal reflectance of the proposed structure 1D an eight-layer (Si/SiO_2) (b) Normal reflectance of the modified structure, for TM waves

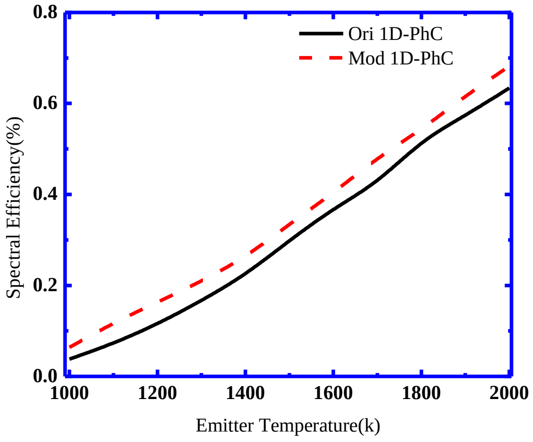


Fig.4 Spectral efficiency of TPV systems as function of the emitter temperature with, the original PhC (solid line), and the modified 1D PhC (dashed line) for TM wave

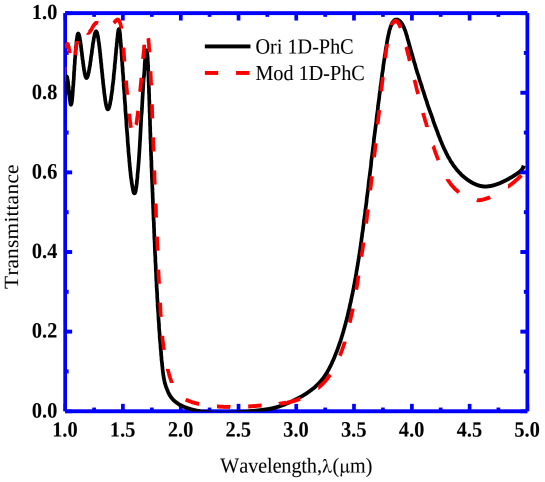


Fig.5Normal transmittance of the original proposed and modified structure for TM waves

6.2 Effect of the Incidence Angle on the Reflectance

The effect of incidence angle on the reflectance of the original structure and modified structure is studied with different incidence angles. The reflectance of the original proposed structure and modified structure for TM waves is shown in Fig.6. It can be seen that when the incident angle increases, the spectral reflectance decreases in pass-band region. The stop band shifts a little toward short wavelength with the increase of the incident angle. We notice that the modified structure has lower reflectance than the original proposed structure in the pass band region.

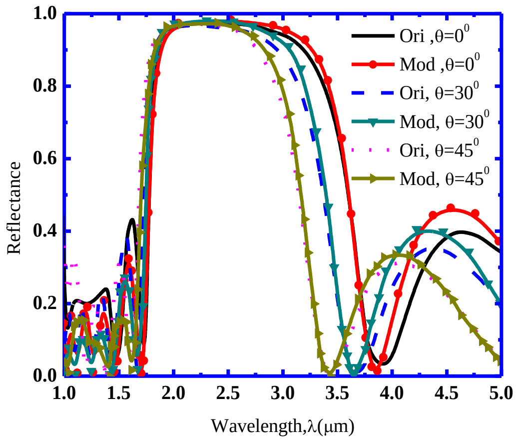
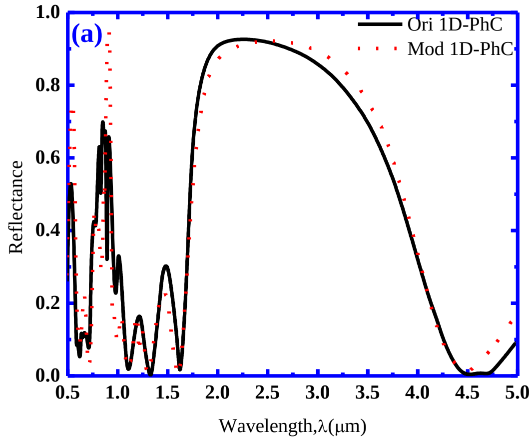


Fig.6Reflectance of the original proposed and the modified structure with different incidence angles for TM waves

6.3Effect of the Number of Periods on the Reflectance

The normal reflectance of the, original structure and modified structure as obtained by the RCWA method for TM waves with different periods shown in Fig.7.It can be observed that as the period increases, the dip shifts toward longer wavelength for photons at $\lambda<1.73\mu m$ and shorter wavelength at $\lambda>1.73\mu m$. The stop band becomes narrow and higher reflectance with increases number of periods. It can be seen that 1DPhC modified structure has flatter and lower pass band compared with the original proposed in all below figures. Note that the spectral reflectance affected by a number of layers of PhC.



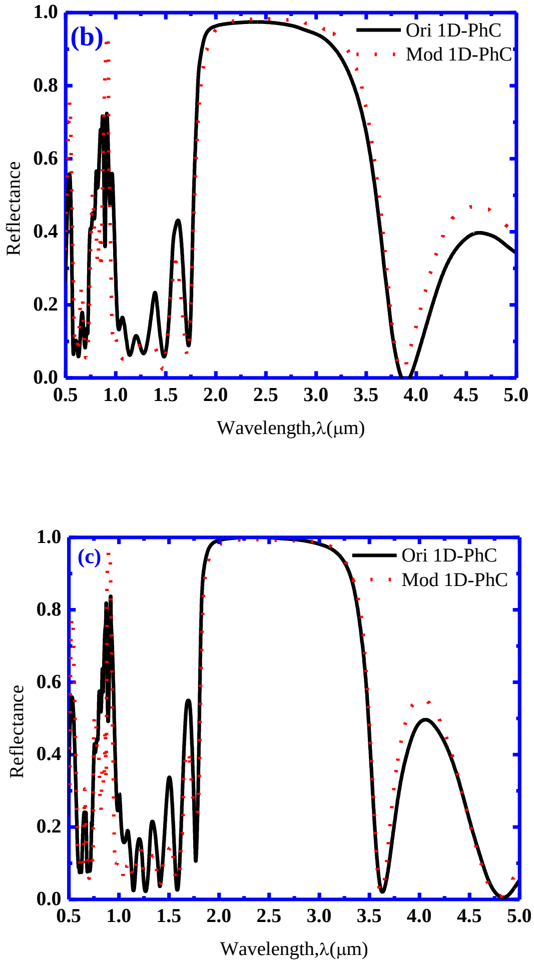


Fig.7 Normal reflectance of the original proposed and the modified structure for TM waves with different period (a) P=3 (b) P=4 (c) P=5

A spectrophotometer (U- 4100, Hitachi Co.) was used to measure the normal reflectance of the prepared 1DSi/SiO_2 PhCs at a wavelength range 0.5-3 μm and shown in Fig.8.The measured results are in good agreement with the simulated results, while the measured is a little higher than that the simulated results. This is mainly because in the simulation we used the thickness of the quartz substrate is infinite while the actual thickness of the quartz substrate is limited in measurement. The experiment and simulated results indicated that the modified 1D PhC exhibits a much flatter and lower pass band compared with the original proposed 1DPhC.

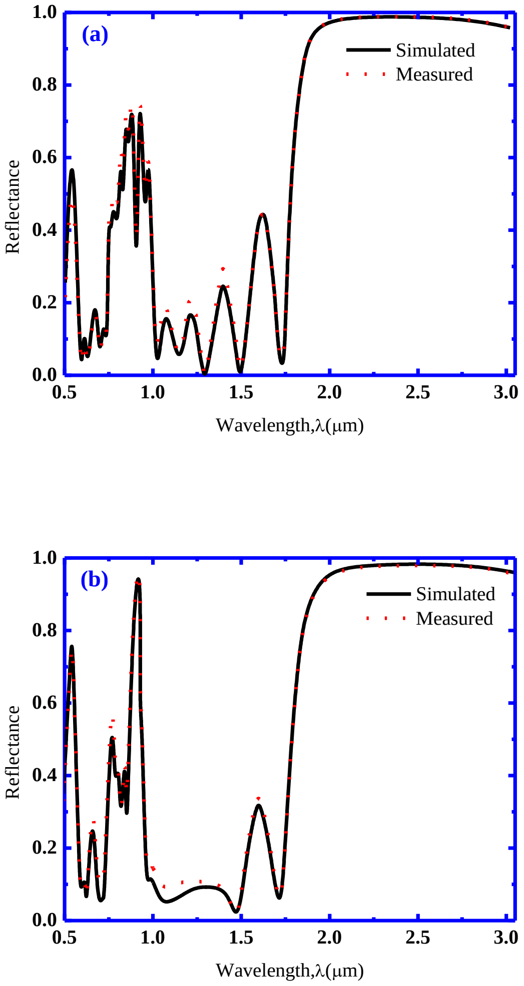


Fig.8 Measured and simulated normal reflectance of (a) the original proposed 1DPhC (b) The modified 1DPhC for TM waves

7 Conclusion

In the present work, we have studied a one - dimensional photonic crystal (1D Si/SiO_2 PhC), for design and development of a spectrally selective filters that are to be used in TPV applications. The influence of layers geometric parameters on the reflectance and spectral efficiency of the filter is studied by using the rigorous coupled-wave analysis (RCWA). The effect of the incident angles on the spectral reflectance also was discussed. The modified structure recycles most of the unconvertible photons in the wavelength region $1.73\mu m < \lambda < 3.9\mu m$ utilizing the stop band, which would greatly improve the system performance. The spectral efficiency value of the modified structure is 33.5%at emitter temperature of about $1500\,K$. The experiment and simulated results indicated that the modified 1D PhC exhibits a much flatter and lower pass band compared with the original proposed 1DPhC.

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