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Investigation of one-dimensional Si/SiO_2 photonic crystals for thermophotovoltaic filter

LIU GuangPing, XUAN YiMin†, HAN YuGe & LI Qiang

School of Power Engineering, Nanjing University of Science & Technology, Nanjing 210094, China

The spectral control is widely incorporated with the thermophotovoltaic (TPV) technology to improve the optical-electric conversion efficiency of the whole system. In order to match with GaSb photovoltaic cell, an 8-layer one-dimensional photonic crystals (PC) filter structure was designed as quarter-wave periodic structure by selecting silicon (Si) and silicon dioxide (SiO_2) as candidate materials. The multilayer Si/SiO_2 structure was developed for the matching filter to simultaneously realize the optimal matching with the spectral distribution of the high temperature emitter and the quantum efficiency of GaSb cell. The physical vapor deposition (PVD) method was used to fabricate the optical filter and the normal incidence optical property of the filter was measured within the spectral range from 0.7 to 3.3 μm. These experimental data were used to predict the spectral control performance in a TPV system. Finally, temperature performance experiments were carried out to establish its withstanding performance in high temperature environment.

spectral filter, optical property, thermophotovoltaics, one-dimensional photonic crystals

The thermophotovoltaic (TPV) technology is a new promising approach that directly converts the radiated thermal energy emitted from a high temperature emitter into electricity using the photovoltaic effects of semiconductor materials[1,2]. Although the concept of TPV was first proposed in 1960s, some defects and difficulties in semiconductor trapped its developments. Until the 1990s rapid progresses in III-IV semiconductor materials with low band gap energy greatly stimulated the developments of TPV technology. Recently, more and more efforts have been concentrated on improving the optical-electrical conversion efficiency and application issues of a TPV system.

The investigation on a TPV system mainly focuses on increasing its conversion efficiency and power density. For such purpose, the spectral control of thermal radiation from an emitter to a

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†Corresponding author (email: ymxuan@mail.njust.edu.cn)
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photovoltaic cell is a vital and practical approach. One of the effective approaches for the spectral control is to use a filter device for controlling photons selectively from an emitter to a photovoltaic cell. The filter device in a TPV system plays its role in the following two aspects: (1) To recycle thermal radiation, i.e. to reflect photons whose wavelengths are above the band gap wavelength of a photovoltaic cell back to the emitter, which helps to maintain the high temperature level of the emitter and reduce the cooling load of the photovoltaic cell. (2) To transmit photons selectively, i.e. to let the photons from an emitter whose wavelengths are below the band gap wavelength of a photovoltaic cell penetrate the filter and reach the cell. These photons can be absorbed and stimulate electrons out of the photovoltaic cell. The demand of developing suitable filter device stimulates further investigation efforts to improve the conversion efficiency of TPV system. Several research groups have been devoting their work to filter exploration with its performance improvement, and several typical filter structures have been proposed including the plasma filter[3−5], one-dimensional PC[6,7] filter, and the frequency selective surface[8,9].

One-dimensional PC is a type of functional structure for spectral control in a TPV system and its most attractive advantage is its simple structure which could be fabricated easily. Sullivan et al.[6,7] proposed a 10-layer one-dimensional Si/SiO_2 PC filter structure which showed high spectral control efficiency and the feasibility that the one-dimensional PC filter can be used for spectral control application in a TPV system. The Si/SiO_2 system is one of the excellent candidate material pairs for fabricating one-dimensional PC filter, and its advantages include having a large dielectric index contrast between two adjacent Si/SiO_2 layers, with omnidirectional band gap characteristic[9] and showing the low absorption feature in the near infrared range[11].

The reported one-dimensional Si/SiO_2 PC filter[6,7] mostly focuses on its matching performance with band gap wavelength of the GaSb photovoltaic cell, i.e. the filter is required to reflect the photons above the band gap wavelength and transmit the photons below the band gap wavelength. In fact, transmission performance for the photons whose wavelengths are below the band gap wavelength is very complicated, and matching performance with the spectral distribution of the high temperature emitter and the quantum efficiency of GaSb photovoltaic cell directly affects the optical-electric performance. At the same time, fabrication technique for the one-dimensional Si/SiO_2 PC filter structure may induce some influences on its spectral control performance in a TPV system. If the distance between the high temperature emitter and the filter in a TPV system is very limited, the temperature withstanding performance of the spectral filter device is also vital for the optical-electric conversion.

This study concerned the detailed exploration of one-dimensional PC filter for spectral control in a TPV system, and the filter structure was designed by using Si and SiO_2 material system. The multilayer Si/SiO_2 filter structure was required to realize simultaneously the optimal matching with the spectral distribution of a high temperature emitter and the quantum efficiency of GaSb photovoltaic cell. The physical vapor deposition (PVD) process was used to fabricate the optical filter and its optical properties were experimentally measured. Finally, the experimental data were used for estimating spectral control performance.

This article is organized as follows. In section 1 the one-dimensional Si/SiO_2 PC filter structure is designed and optimized in the light of the electromagnetic wave theory to maintain the spectral matching with the band gap energy of the GaSb photovoltaic cell used in a TPV system. In addition, the optical properties of the filter are simulated and analyzed. In section 2 the optimization of the multilayer filter is to simultaneously realize the optimal matching with the spectral distribution of the high temperature emitter and the quantum efficiency of GaSb cell, and is conducted to improve and enhance its transmission performance. In section 3 the fabrication procedure of the one-dimensional Si/SiO_2 PC structure is involved and its optical properties are measured. The spectral control performance of the one-dimensional Si/SiO_2 PC filter is estimated from the measured data. In section 4 an overview is given.

1 Design of one-dimensional Si/SiO_2 PC filter

Here the TPV system consists of three devices including an emitter, a filter, and a GaSb photovoltaic cell. Figure 1 shows the schematic diagram of the TPV system. The high temperature emitter is assumed to be a blackbody and the GaSb photovoltaic cell corresponds to the band gap energy 0.72 eV and band gap wavelength 1.8 μm, respectively. The optical filter is placed in front of the GaSb photovoltaic cell. The Si and SiO_2 material system for the filter is expressed with H (high refractive index material) and L (low refractive index material), respectively. The absorption losses of the two materials are close to zero in the wavelength range above 0.5 μm[10], so their refractive indexes are considered to be n_H=3.4 for Si and n_L =1.47 for SiO_2 in the design calculation[10], respectively. The substrate material for the filter is quartz and its refractive index is equal to 1.5.

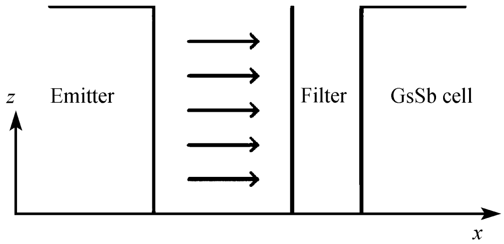

Figure 1 Schematic diagram of a TPV system consisting of a high temperature emitter, a filter device, and a conversion cell.

One-dimensional Si/SiO_2 PC structure is essentially a quarter-wave periodic multilayer film. While a beam of light (i.e. a number of photons) penetrates the periodic structure, the interference process is enhanced. This process synthetically leads to the high transmission and high reflection for the photons. So according to propagation of light in media and quarter-wave film theory, it is easy to derive the equation in terms of the band-gap central wavelength λ_0 and the lower edge λ_b of the high reflection band as follows[6]:

$$\lambda_0 = \frac{1}{1-\dfrac{2}{\pi}\sin^{-1}\left(\dfrac{n_H - n_L}{n_H + n_L}\right)}\lambda_b. \tag{1}$$

The thickness of dielectric layer is given as

$$d_i = \frac{\lambda_0}{4n_i}, \tag{2}$$

where i represents H and L.

One-dimensional Si/SiO_2 PC filter structure was designed as $(LH)_4$. We substituted the optical parameters of Si and SiO_2 into eqs. (1) and (2) and got thicknesses of Si and SiO_2 layers in one-dimensional PC filter structure as 0.176 and 0.408 μm. The optical properties of the designed filter were simulated by the transfer matrix method (TMM). The simulated results showed that 1.8—3.3 μm and 0.72—0.9 μm were high reflection bands and the maximum reflectivity was close to 1.0, and 0.9—1.8 μm and 0.5—0.72 μm were high transmission bands. At the same time, strong oscillations were in the designed filter's transmission bands in wavelength range below 1.8 μm, and such oscillations heavily reduced transmission of photons in corresponding wavelength ranges.

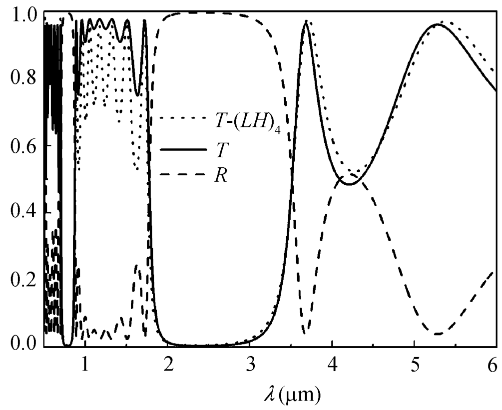

Figure 2 Simulated optical properties of the 8-layer one-dimensional Si/SiO_2 PC filter with $L/2H(LH)_3$ with the transmissivity of $(LH)_4$ structure. T-$(LH)_4$ represents transmissivity of $(LH)_4$ structure. T and R represent transmissivity and reflectivity of $L/2H(LH)_3$ structure, respectively.

An effective way of reducing such oscillations is to use a filter with $L/2H(LH)_3$ structure instead of the original design structure $(LH)_4$, i.e. the thickness of SiO_2 layer in the first period unit is reduced to 0.204 μm. The optical properties of the $L/2H(LH)_3$ filter structure were calculated and given in Figure 2 with those of the $(LH)_4$ structure, where the T-$(LH)_4$ is transmissivity of the $(LH)_4$ structure, R and T represent reflectivity and transmissivity, respectively. The only difference between the spectral properties of the two structures is that transmissivities of $L/2H(LH)_3$ structure in 0.9—1.8 μm range are enhanced to the average of 0.92. At the same time, there is a transmittance trough locating in 1.5—1.8 μm range, which also reduces transmission of photons in the wavelength range. In addition, the photons losses in Si layers of the filter are very strong and cannot be neglected in the wavelength below 0.5 μm[11], so photons emitted by high temperature emitter in the wavelength range can be absorbed by the filter structure.

2 Improving transmission performance

One-dimensional Si/SiO_2 PC filter shows its reflection and transmission performance in a TPV system with GaSb cell. Excellent reflection performance means that the filter structure has the reflection band as wide as possible and possibly a higher reflectivity close to 1.0 for the photons over the band gap of the GaSb conversion cell. The reflection performance of the filter is dependent upon its structure size and features of the materials such as contrast of refractive indexes of high and low dielectric materials and total layers of candidate materials. One-dimensional Si/SiO_2 PC filter structure should transmit photons below the band gap wavelength of GaSb photovoltaic cell as many as possible. Actually, the transmission performance of the filter is complicated and its design must account for the following two issues: the spectral distribution of thermal radiation from the high temperature emitter and the quantum efficiency of GaSb photovoltaic cell.

2.1 Spectral distribution of high temperature emitter

One of the important issues for improving the spectral transmission performance of the one-dimensional Si/SiO_2 PC 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. According to the Planck law, the spectral radiation power of high temperature source is expressed as[12]

$$E(\lambda,T)=\frac{C_1}{\lambda^5\left[\exp(C_2/\lambda T)-1\right]},\tag{3}$$

where $C_1=3.742\times10^8\ \mathrm{W\cdot\mu m^4/m^2}$, and $C_2=1.439\times10^4\ \mathrm{\mu m\cdot K}$. The spectral radiation power was calculated from eq. (3) with temperatures being 1300, 1400, 1500 and 1600 K, respectively.

The results corresponding to the wavelength range below 2.0 μm were given in Figure 3. Even though the temperature of high temperature source reaches 1600 K, the total radiation power in 0.5—0.72 μm range is less than 1.7% of that in 0.5—2.0 μm range. Figure 3 suggests that total radiation power in 0.5—0.72 μm range is very limited, so photons reaching GaSb photovoltaic cell mostly locate in the wavelength range of 0.9—1.8 μm. In order to realize this issue further, the 0.9—1.8 μm range was divided into two wavelength ranges, i.e. 0.9—1.4 μm and 1.4—1.8 μm. Here, the radiation power ratio was defined as the ratio of total radiation power in 1.4—1.8 μm range to that in 0.9—1.8 μm range. Variation of the radiation power ratio with the temperature level of an emitter is indicated in Figure 4. For the case that the temperature of an emitter was below 1800 K, the radiation power ratio was over 50%, indicating that most of the radiation power from an emitter was limited in the spectral range of 1.4—1.8 μm. Thus, the design of the filter should ensure this wavelength band to be its high transmission band.

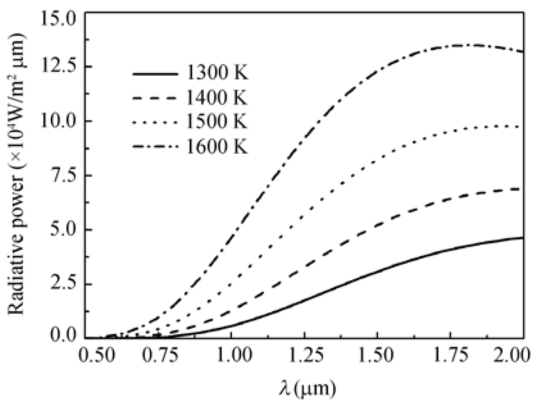

Figure 3 Spectral distribution power radiated from an emitter in 0.5—2.0 μm range.

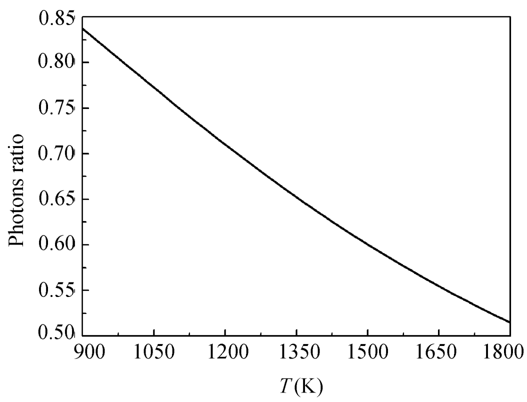

Figure 4 Variation of the radiation power ratio with the temperature level of an emitter.

2.2 Quantum efficiency of GaSb photovoltaic cell

It includes two issues for one-dimensional Si/SiO_2 PC filter to match well with GaSb photovoltaic cell. First, high reflection band and high transmission band of the filter should match with the band gap wavelength of GaSb photovoltaic cell, i.e. the filter should reflect photons whose wavelengths are over 1.8 μm back to the high temperature emitter. Second, transmission of the photons in wavelength below 1.8 μm through the filter should match well with the quantum efficiency of GaSb photovoltaic cell, i.e. the filter should transmit photons as many as possible in the wavelength range corresponding to the high quantum efficiency of GaSb photovoltaic cell. The quantum efficiency of GaSb photovoltaic cell expresses its absorption and conversion ability of photons in wavelength below 1.8 μm. The measured quantum efficiency of GaSb photovoltaic cell can be found elsewhere[13] which makes it clear that most of the photons in the wavelength range of 0.5—1.8 μm can be absorbed and converted into electricity by GaSb photovoltaic cell. So spectral transmission performance of one-dimensional Si/SiO_2 PC filter in the wavelength range of 0.9—1.8 μm must simultaneously match with the spectral distribution of the emitter and the quantum efficiency of GaSb photovoltaic cell in order to realize the maximal conversion efficiency and power density in TPV system.

2.3 Improvement of one-dimensional Si/SiO_2 PC filter structure

The simulated results showed that transmission properties of one-dimensional Si/SiO_2 PC filter in 0.9—1.8 μm range were obviously modified by adjusting the thickness of the Si layer in the first period unit. When its thickness was reduced based on design value 0.176 μm, transmissivity became lower in 1.4—1.8 μm range but higher in 0.9—1.4 μm range, and the opposite results were gained in the two wavelength ranges by increasing its thickness based on 0.176 μm. Taking into account one-dimensional Si/SiO_2 PC filter matching with photons spectral from emitter and the quantum efficiency of GaSb photovoltaic cell, we got the matching filter structure with excellent transmission performance in the wavelength range of 0.9—1.8 μm by adjusting the thickness of the Si layer in the first period unit to 0.194 μm. The optical properties of the matching filter structure were simulated by TMM and compared to those of the $L/2H(LH)_3$ structure. The compared results were shown in Figure 5, where the transmissivity of the matching filter for the photons in 1.4—1.8 μm range was improved from 72% to 85%. On the other hand, transmissivity in 0.9—1.4 μm range was reduced and some slight oscillation could be seen, which might be negligible compared to transmission performance improvement of the filter in 1.4—1.8 μm range. The improved transmission performance was shown in Figure 6 with the quantum efficiency of GaSb photovoltaic cell.

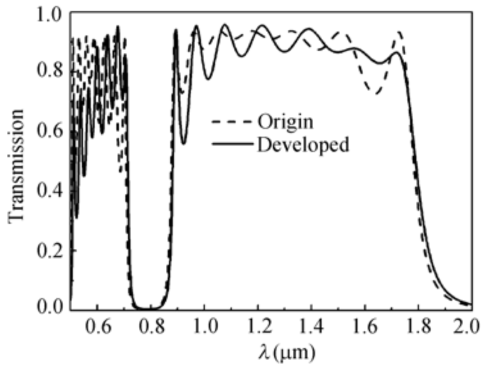

Figure 5 Comparison of transmission properties of the two filter structures. ‘Origin’ represents the designed 8-layer $L/2H(LH)_3$ PC filter structure, with the thickness of SiO_2 and Si being 0.204 and 0.176 μm in the first period unit, and 0.408 and 0.176 μm in the other three period units. ‘develop’ represents the matching PC filter structure, with the thickness of SiO_2 and Si being 0.204 and 0.1944 μm in the first period unit, and 0.408 and 0.176 μm in the other three period units.

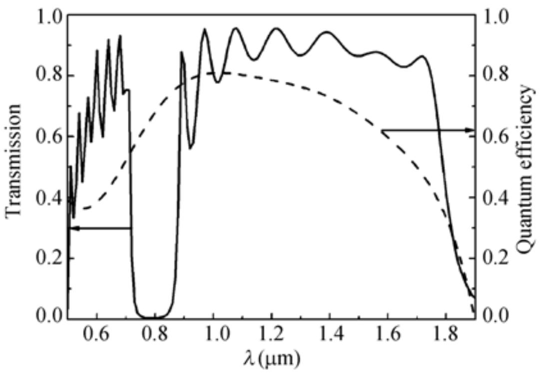

Figure 6 Improved transmission performance of the matching Si/SiO_2 PC filter in 0.5—1.9 μm range with the corresponding quantum efficiency of GaSb photovoltaic cell.

3 Fabrication of filter structure

The PVD method is one of the advanced optics vacuum coating technologies and is widely used to fabricate optics multilayer film. It was used to fabricate the matching one-dimensional Si/SiO_2 PC filter. A sample of the matching filter is shown in Figure 7 and its size is 50 mm×25 mm×2 mm. The normal optical properties of the 8-layer matching filter were measured in two different wavelength ranges of 0.7—1.1 μm by using spectrophotometer UV-2802 and 1.0—3.3 μm with spectrophotometer $\lambda-900$, respectively. The experimental results were compared with the simulated ones based on the Maxwell’s electromagnetic theory as shown in Figures 8 and 9, respectively. Obviously, the fabricated filter provided the high reflection performance corresponding to the wavelength range of 1.8—3.3 μm with reflectivity of 0.92 and the high transmission corresponding to 0.9—1.8 μm with the averaged transmissivity of 0.9. The somewhat slight differences in the nearby range of 1.0 μm could be observed from Figures 8 and 9, which resulted from the instrument error of these two spectrophotometers.

Figure 7 Sample of one-dimensional PC Si/SiO_2.

The spectral efficiency of the matching filter was calculated with the measured spectral properties to estimate the effect of the spectral control of the fabricated 8-layer one-dimensional Si/SiO_2 PC filter in a TPV system (as shown in Figure 10). Here, the spectral efficiency of the filter was defined elsewhere[6]. When the emitter temperatures were 1300, 1400, 1500 and 1600 K, the predicted spectral efficiencies of the 8-layer one-dimensional Si/SiO_2 PC filter corresponded to 31%, 37%, 46% and 53%, respectively, which was 8% higher than those of the 10-layer one-dimensional Si/SiO_2 PC filter[6]. Such improvement of the spectral efficiency was due to the fact that the fabricated 8-layer filter possesses a better transmission feature within the wavelength range of 0.9—1.8 μm.

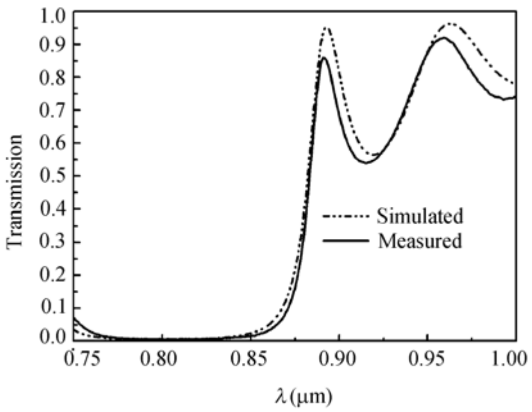

Figure 8 Comparison of transmissivity of the 8-layer matching filter in 0.7—1.0 μm range.

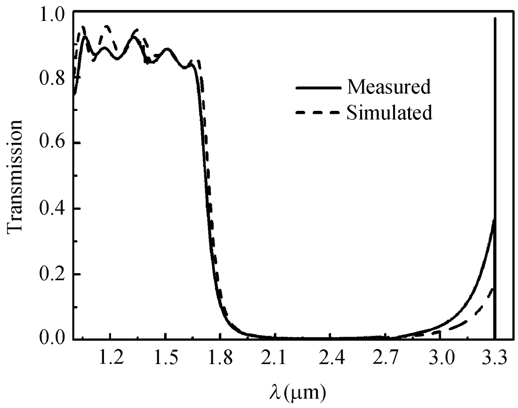

Figure 9 Comparison of transmissivity of the 8-layer matching filter in 1.0—3.3 μm range.

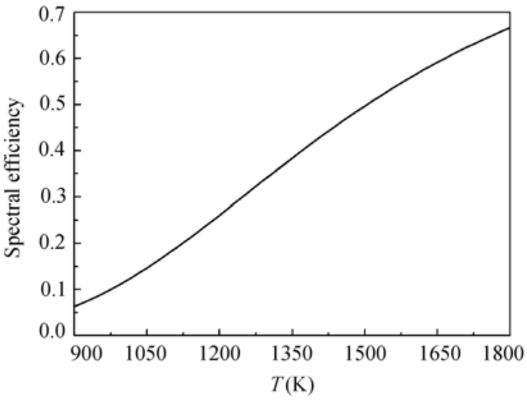

Figure 10 Spectral efficiency of the 8-layer matching one-dimensional Si/SiO_2 PC filter in TPV system.

As described above, the filter is effective for spectral control and its performance directly exerts influences onto the optical-electric conversion in a TPV system. The optical-electric conversion performance can be scaled by the system efficiency and power density which were defined elsewhere[6]. The system efficiency and power density of the TPV system with a 8-layer matching one-dimensional Si/SiO_2 PC filter were predicted, which were illustrated in Figures 11 and 12.

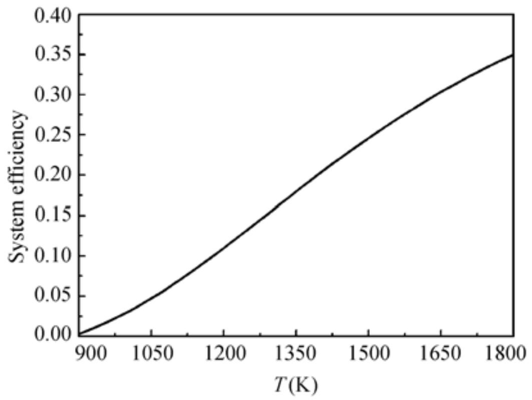

Figure 11 The predicted system efficiency of TPV system with the matching 8-layer one-dimensional Si/SiO_2 PC filter structure.

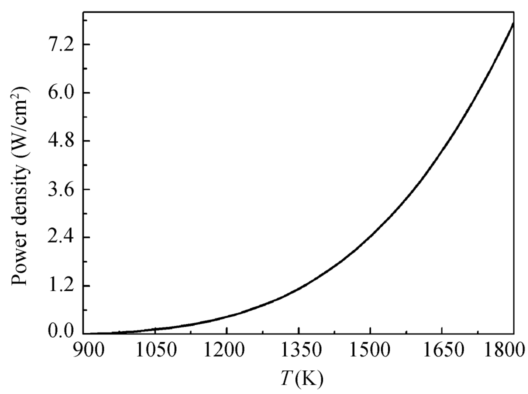

Figure 12 The predicted power density of TPV system with matching 8-layer one-dimensional Si/SiO_2 PC filter structure.

When the emitter temperatures were 1200, 1400, 1600, and 1800 K, the predicted system efficiencies corresponded to 10.9%, 19.8%, 26% and 35.3%, respectively, and the predicted power densities were equal to 0.589, 1.77, 3.92 and 7.75 W/cm^2, respectively. Compared to the predicted ones of the 10-layer one-dimensional Si/SiO_2 PC filter in ref. [6], the system efficiency of the 8-layer filter was enhanced by 1.7% and the maximum power density increased by 0.8 W/cm^2.

For practical application, the optical filter is usually in close proximity to the high temperature emitter, so it is necessary to estimate the temperature-withstanding performance of the fabricated 8-layer matching one-dimensional Si/SiO_2 PC filter. The experiment was conducted for different temperatures in which the fabricated filter was heated to 400℃, 500℃, 600℃, and 700℃ for 4 h, respectively. Then, the optical properties were immediately measured and the four experimental data were compared with the optical properties at the room temperature of 30℃. The comparison showed the filter's satisfactory consistency of the transmission feature for the different temperature levels except that at 700℃. When the filter was heated to 700℃ for 4 h, its measured result showed that its transmission feature shifted 0.2 μm toward the short wavelength as a whole (as shown in Figure 13). Such a transmission shift of the filter may reduce the photons reaching the surface of GaSb photovoltaic cell and cause degradation of the optical-electric conversion of the TPV system. Therefore, we can conclude that the 8-layer matching one-dimensional Si/SiO_2 PC filter can safely work below 600℃.

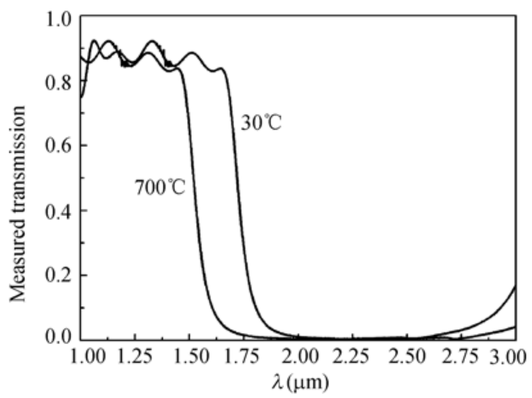

Figure 13 Measured transmission performance of the fabricated filter at 700 and 30℃, respectively.

4 Overview and conclusion

We have developed the one-dimensional PC filter for the spectral control of photons in order to maximize the conversion efficiency and power density of a TPV system. The filter structure has been designed as 4 periods and 8 layers (4 pairs) by using SiO_2 and Si material pair, and the thicknesses of SiO_2 and Si layer have been determined to be equal to 0.204 and 0.194 μm in the first period and 0.408 and 0.176 μm in the other three periods. The PVD process has successfully been used to fabricate the filter. The normal transmittance performance of the filter has been measured with two spectrophotometers within the spectral range from 0.7 to 3.3 μm. It shows that the reflectivity of the filter is over 92% in the wavelength range 1.8—3.3 μm and the averaged transmissivity reaches 90% in the wavelength range 0.9—1.8 μm. The theoretical prediction has also given the identical results. The estimated spectral efficiency of the TPV increases with the emitter temperature. For example, the spectral efficiency of the TPV system with such a filter reaches 53%. The temperature-withstanding experiment has indicated that the fabricated 8-layer matching one-dimensional $SiSiO_2$ PC filter can normally work at the temperature environment below 600℃.

One-dimensional PC filter shows its advantages of simple structure and fabrication process and can be conveniently applied to spectral control of the TPV system. It has been found that the filter has the satisfactory transmission performance within the wavelength range of 0.9—1.8 μm with respect to the simultaneous spectral matching of the filter with both the spectral distribution of the high temperature emitter and the quantum efficiency of GaSb photovoltaic cell.

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