1D and 2D Photonic Crystals for Thermophotovoltaic Applications

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ABSTRACT

This paper explores the optical characteristics of one-dimensional (1D) and two-dimensional (2D) photonic crystals (PhC) as spectral control components for use in thermophotovoltaic (TPV) systems. 1D PhC are used as optical filters while 2D PhC are used as selective thermal emitters. A Si/SiO_2 1D PhC is fabricated using low-pressure chemical vapor deposition (LPCVD). The measurement and characterization of this structure is presented. A 2D hexagonal PhC of periodic holes is fabricated using interference litography and reactive ion etching (RIE) process. Our results predict that a TPV system utilizing a 2D PhC selective emitter and 1D Si/SiO_2 PhC optical filter promises significant performance improvements over conventional TPV system architectures.

Keywords: Thermophotovoltaics, photonic crystal, thermal emission

1. INTRODUCTION

Thermophotovoltaics (TPV) are static energy converters that convert thermal radiation into electricity by means of a photovoltaic (PV) diode[1−3]. The TPV device consists of an emitter, a PV diode and a spectral control component (filter). The emitter converts heat into radiation (mostly in the near infra-red), which is selectively filtered by an optical filter. Part of the radiation is transmitted to the PV diode and the rest is reflected back to the emitter. The PV diode converts the transmitted photons with energies in excess of the diode bandgap energy into charge carriers, while the photons below the bandgap energy are partially absorbed and converted into waste heat and partially reflected back to the emitter by the back side contact.

Although, the concept of TPV power conversion was first proposed in the 1960s,[1] it has only recently been practical to consider it as a viable power conversion technology for many commercial, space and military applications. This is due to the fact that recently there have been significant technological advancements in the areas of low-bandgap semiconductor materials (such as GaSb, InGaAs, InGaAsSb or similar), optical components and photonic crystals. In particular, there has been a significant amount of work carried out on low-bandgap materials for TPV applications[4,5]. A similar body of work does not yet exist with regards to spectral control and the application of photonic crystals in TPV systems. Therefore, we focus our attention on improving the performance of TPV systems through the use of photonic crystals. In this article we investigate the performance of one-dimensional (1D) and two-dimensional (2D) photonic crystals (PhC) as spectral control components for TPV applications. We will analyze how 1D and 2D PhCs influence TPV system efficiency and power density and what the design constraints are.

2. THERMOPHOTOVOLTAIC SYSTEM MODELLING

In this paper we analyze a TPV system that consists of an emitter and a PV diode. A 1D PhC is deposited on the front side of the PV diode and this is separated from the emitter by a gap as shown in Fig. 1. The performance of the TPV system is assessed with respect to the efficiency and power density delivered by the PV diode using the ideal thermodynamic model described in[5,6]. We assume that the PV diode is a GaSb device (with an electronic bandgap of $E_g = 0.7$ eV corresponding to a wavelength of $\lambda_g = 1.78$ μm and with refractive

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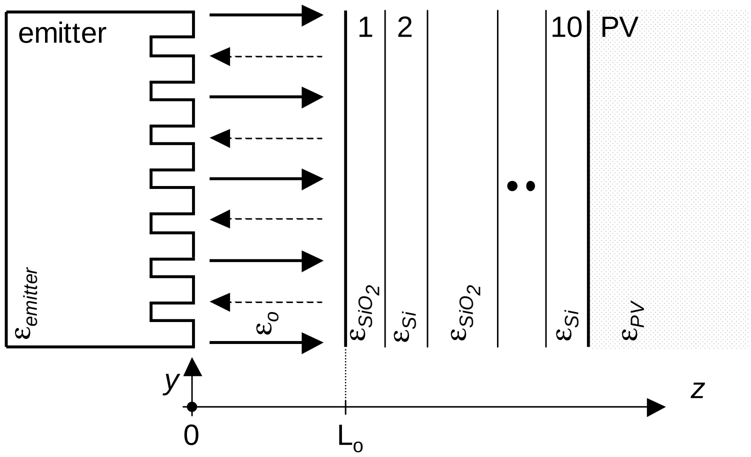

Figure 1. TPV system with 2D photonic crystal as selective emitter and a front side dielectric stack filter (1D PhC) deposited on the PV diode that extends to $+\infty$.

index $n = 3.9$). In addition to the PV diode efficiency and power density, spectral efficiency is used as a figure of merit for assessing the performance of both the selective emitter and the filter. Spectral efficiency can be defined as[4]:

$$\eta_{spectral}(T_{BB}, \omega_g, T_{PV}) = \frac{\int_0^{\omega_g} \frac{\omega^2}{(2\pi)^2 c^2} \frac{\hbar\omega}{\exp(\frac{\hbar\omega}{kT_{BB}})-1} \varepsilon_{emitter}(\omega) T_{filter}(\omega) d\omega}{\int_0^{\infty} \frac{\omega^2}{(2\pi)^2 c^2} \frac{\hbar\omega}{\exp(\frac{\hbar\omega}{kT_{BB}})-1} \varepsilon_{emitter}(\omega)(1 - R_{filter}(\omega)) d\omega}, \tag{1}$$

where $T_{filter}(\omega)$ is the average angular transmittance of the filter (including both TE and TM transmittances), $R_{filter}(\omega)$ is the average reflectance of the filter and $\varepsilon_{emitter}(\omega)$ is the hemispherical emittance of the thermal source. Spectral efficiency, as defined in Equation (1), gives the ratio of the above bandgap transmitted power to the total emitted power that reaches the diode-filter system. Spectral efficiency can therefore be engineered by tailoring either $T_{filter}(\omega)$ or $\varepsilon_{emitter}(\omega)$ or both.

Ideal spectral control can be achieved with the blackbody source ($\varepsilon_{emitter}(\omega) = 1$) and an ideal filter. Such a filter transmits all the above bandgap photons to the PV diode ($T_{13} = 1$ for $\omega > \omega_{\text{gap}}$) while reflecting all lower energy photons ($T_{13} = 0$ for $\omega < \omega_{\text{gap}}$) back to the source. Achieving such ideal spectral control is not possible however, this paper will show that the use of a multi-period Si/SiO_2 structure combined with a 2D PhC selective emitter can provide enviable spectral efficiency and system performance.

3. 1D SI/SIO_2 PHOTONIC CRYSTAL

A 1D PhC does not exhibit a complete photonic bandgap however, when coupled to free space it does exhibits total omnidirectional reflectance[7,8] . In our design we utilize this omnidirectional reflectance band of a quarter-wave 1D Si/SiO_2 PhC deposited on front side of PV diode to improve efficiency. The central wavelength of the normal-incidence stop-band is given as:

$$\lambda_0 = \frac{1}{2}\left(1 + \frac{2 + \frac{4}{\pi}\sin^{-1}\frac{n_2 - n_1}{n_2 + n_1}}{2 - \frac{4}{\pi}\sin^{-1}\frac{n_2 - n_1}{n_2 + n_1}}\right)\lambda_g, \tag{2}$$

where λ_g is the normal incidence bandgap edge, and $n_1 = 1.5$ and $n_2 = 3.4$ are the refractive indices of SiO_2 and Si respectively. We designed the 1D PhC for use with a GaSb PV diode ($\lambda_g = 1.78$ μm). Therefore, by substituting this into Equation (2) we calculate λ_0 which is the central wavelength of photonic bandgap. Our photonic crystal is based on a quarter wave stack, and therefore,

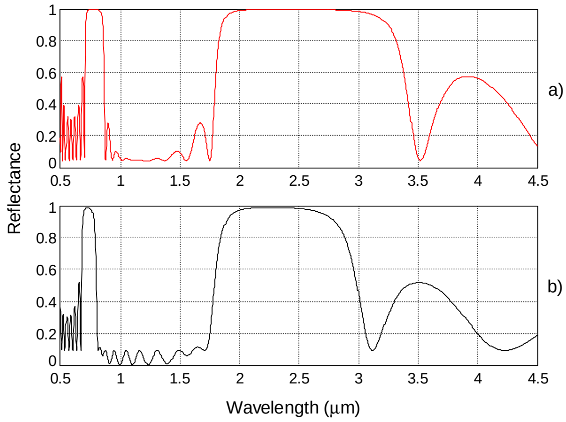

Figure 2. Reflectance of ten-layer $\frac{L}{2}H(LH)^4$ Si/SiO$_2$ and Si/SiON quarter-wave stack photonic crystal.

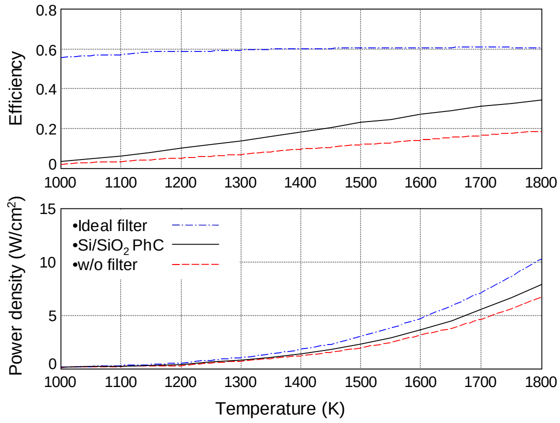

Figure 3. Simulated system efficiency and power density of GaSb TPV system vs. the emitter temperature with an ideal filter, with ten-layer Si/SiO$_2$ filter and without any filter.

$$\lambda_0 = 4n_1d_1 = 4n_2d_2. \tag{3}$$

From Equation (3) the layer thicknesses were found to be $d_1 = 0.39$ μm and $d_2 = 0.17$ μm respectively. Indeed, the normal incidence reflectance of a ten layer (LH)^5 structure deposited on a Si substrate exhibits wide stop-band, however, large oscillations in the pass-band ($\omega > \omega_{\text{gap}}$) significantly reduce the amount of power transmitted to the PV diode. The easiest way to increase the passband transmittance is to use a $\frac{L}{2}H(LH)^4$ PhC structure instead. This only requires modifying the last L layer, reducing its thickness to half its origional thickness, which can then be thought of an anti reflection coating (ARC). The simulated normal incidence reflectance for this structure is given in Fig. 2 a). The passband performance can be further improved—as shown in Fig. 2 b)—by using a $\frac{L}{2}H(LH)^4$ Si/SiON PhC structure. The improved passband performance is the result of better matching of the refractive indices of the PhC to the substrate. Unfortunately, this reduces the width of the stopband.

To evaluate the performance of a 1D PhC deposited on the front side of a GaSb PV diode we simulated the TPV system efficiency, power density and spectral efficiency as a function of the source temperature assuming a blackbody emitter with: (1) a 1D PhC filter, (2) no filter and (3) an ideal filter. The results are shown in Fig. 3. The efficiency of the TPV system using the 1D PhC is more than two times that of the system without any filter, however, the 1D PhC does cause a reduction in power density. Note that all calculations take into account the angular dependance of the filter's reflectance and transmittance.

3.1. Fabrication of 1D Photonic Crystal

The ten-layer Si/SiO$_2$ 1D PhC structures—the design of which is detailed in previous section—were fabricated on p-type Si substrates using a low-pressure chemical vapor deposition (LPCVD) process. In order for the fabricated structures to behave in accordance with what their mathematical models predicted, it was imperative to develop a process, which allowed for very accurate and uniform layer deposition. This process also needed to be relatively low-temperature, given that in the TPV system context the spectral control structure would be directly deposited on the front-side of a GaSb photodiode whose device integrity could not be compromised by the filter fabrication process.

The deposition of the complete ten-layer dielectric stack involved a three step process for the deposition a single Si/SiO$_2$ pair. This was then repeated five times to produce the complete (LH)^5 structure. The first step in the process was the deposition of a poly-Si layer. This layer was grown at 625°C with a SiH$_4$ flow rate of 150 sccm and pressure of 200 mTorr. This was then followed by the deposition of a low temperature oxide (LTO) layer at 400°C with SiH$_4$ and O$_2$ flow rates of 125 sccm and 175 sccm respectively at 200 mTorr pressure. The final step involved a relatively low temperature densification anneal at 650°C for three hours in an N$_2$ ambient

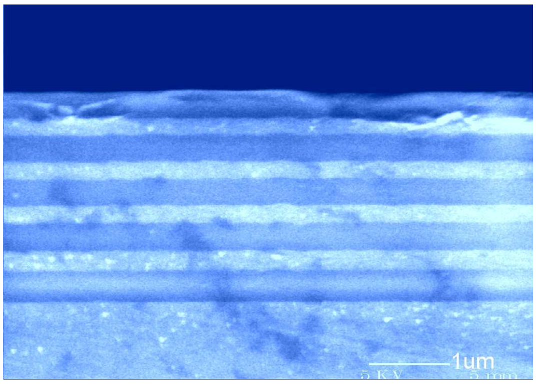

Figure 4. SEM image of the cross section of the ten-layer Si/SiO_2 PhC before half of the top layer (SiO_2) was etched away.

to ensure the quality of the SiO_2 layer. Although the nominal deposition rates for the poly-Si and LTO layers were stated as being 100 Å/min and 53 Å/min respectively a comprehensive set of calibrating deposition runs were carried out prior to the actual dielectric stack fabrication. This procedure identified the actual deposition rates as being equal to 100.1 Å/min and 58 Å/min respectively. Furthermore the calibration process identified the effects of the three-hour anneal on the SiO_2 pair. Specifically a 1744 Å thick poly-Si layer was deposited on a high quality thermal oxide (all thickness measurements were taken using a KLA-Tencor UV-1280 Prometrix Thin Film Thickness Measurement System). A 4115 Å thick layer of SiO_2 was then deposited on top and the dielectric pair was annealed at the stated conditions. After the anneal step the thickness of the Si layer was recorded as being 1675 Å and that of the SiO_2 as being 3535 Å. These results indicated that due to the anneal, the Si layer lost 69 Å due to oxidation, adding 157 Å to the SiO_2 thickness, which therefore meant that the anneal caused an actual reduction in the thickness of the SiO_2 layer of 737 Å. Using this data it was established that in order to ensure the thickness of the Si and SiO_2 layers were 1700 Å and 3900 Å respectively after all the processing steps were completed it was necessary to actually deposit 1769 Å of Si and 4560 Å of SiO_2. In order to produce the final $(LH)^5$ structure the three step process described above was repeated five times.

The fabrication of the modified quarter-wave structure was carried out by etching back the surface layer of the $(LH)^5$ structure to produce a $\frac{L}{2}H(LH)^4$ structure using an Applied Materials Precision 5000 Etcher. The etcher used a CF_4, CHF_3 chemistry and etched the annealed LTO at a rate of 20.6 Å/s.

3.2. Measurement of 1D Photonic Crystal

To insure the quality and uniformity of deposited films we performed measurements of the refractive indices, the layer thicknesses and the surface roughness of the fabricated 1D PhC samples. The refractive indices of the LTO and poly-Si as deposited using LPCVD, and annealed in case of LTO, were measured using a spectroscopic ellipsometer. The measurements were taken across a wavelength range of 250 - 2000 nm. As Fig. 5 illustrates, the measured values matched the reference values[10] very well. Good correspondence of the measured and the reference values illustrates that the LPCVD process is suitable for the fabrication of 1D PhC with high optical quality.

Surface analysis was performed using an atomic force microscope (Digital Instruments Nanoscope IIIa Scanned Probe Microscope). The surface roughnesses of an individual SiO_2 layer and a Si/SiO_2 interface were 20 Å and 40 Å RMS respectively. The RMS roughness of the top surface varied from 60 Å to 90 Å, suggesting that there is some accumulation of roughness with increasing number of layers however, it is well within the acceptable range for this near-infrared application.

A scanning electron microscopy (SEM) was used to examine the cross section of the fabricated structures. The SEM used was a JEOL 6320FV field-emission system. The SEM image of the fabricated structure's cross section—shown in Fig. 4—exhibits excellent layer uniformity and correlates well with the predicted layer thicknesses. The final tests carried out determined the optical response of the 1D PhC. The measured and simulated

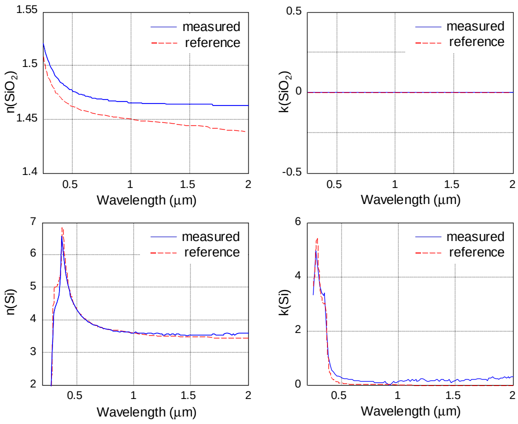

Figure 5. Measured and reference values of the complex refractive indeces of Si and SiO_2.

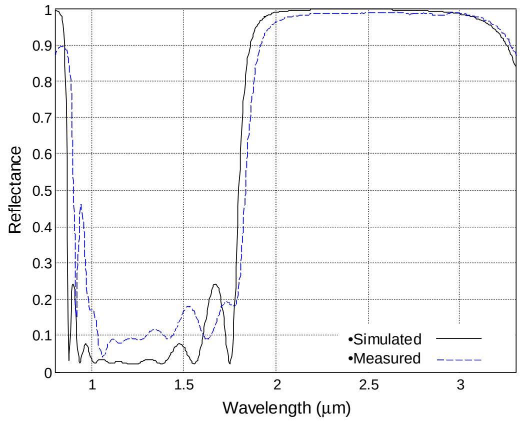

Figure 6. Normal incidence reflectance measurement and simulation results for ten-layer $\frac{L}{2}H(LH)^4$ Si/SiO_2 stack.

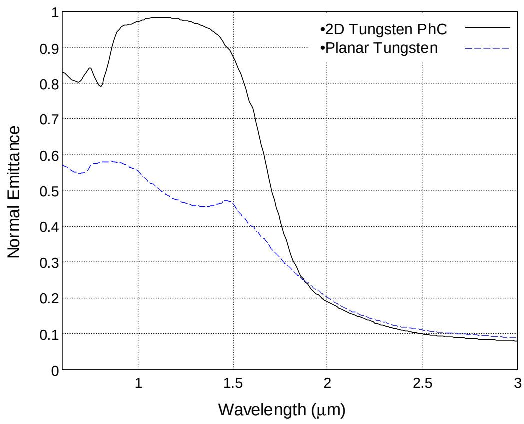

Figure 7. Simulated normal emittance of 2D hexagonal tungsten PhC (with HFSS software, 1 μm periodicity, 800 nm whole diameter and infinite whole depth) and planar tungsten emitter using permitivity values given in Ref. 10.

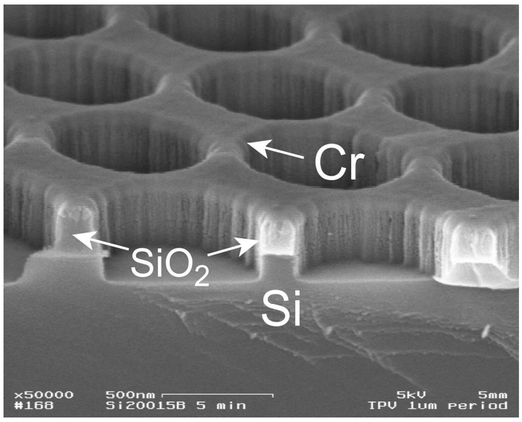

Figure 8. SEM image of partially etched 2D PhC silicon sample with Cr and SiO_2 layers.

reflectance of the ten-layer $\frac{L}{2}H(LH)^4$ structure deposited on the Si substrate, which are shown in Fig. 6 match well, especially in the range of interest from 0.8 - 3.3 μm. Here we have taken into account the effect of the additional reflection from the backside of the Si substrate and the normal reflectance shown in Fig. 6 is re-normalized to the reflectance of the stack on an infinite substrate.

4. 2D PHOTONIC CRYSTAL AS SELECTIVE EMITTER

The 1D PhC as front side optical filter provides excellent spectral control that dramatically improves TPV system efficiency. However, there is still significant room for improvement in terms of matching the radiated spectrum to the PV diode's characteristics in order to approach the ideal spectral control performance necessary to produce very efficient TPV systems. Instead of trying to make the front side optical filter perfect (or nearly perfect) we propose to distribute the spectral control between the emitter and filter. We propose to use a 2D photonic crystal as a selective emitter and combine this with the 1D PhC filter.

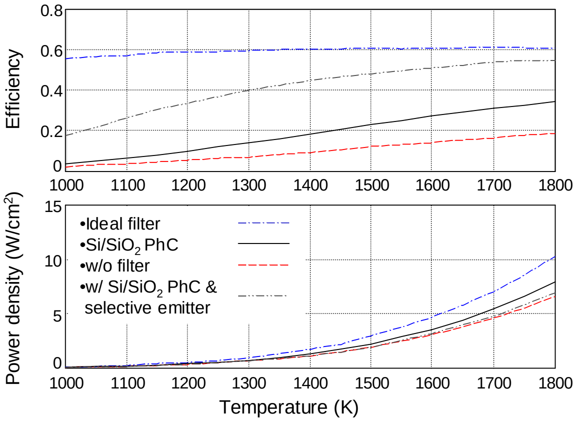

Figure 9. Simulated system efficiency and power density of GaSb TPV system with an ideal filter, ten-layer Si/SiO_2 filter, ten-layer Si/SiO_2 stack and selective emitter, and without any filter vs. the emitter temperature.

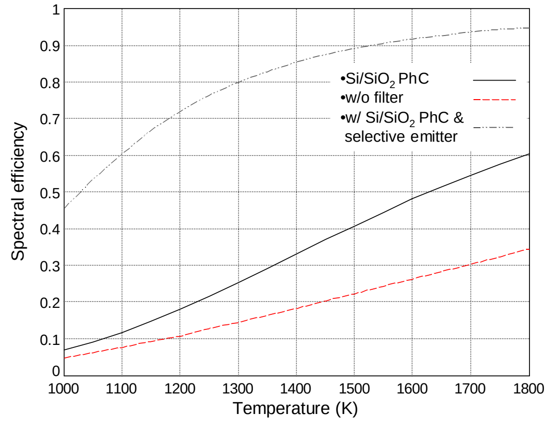

Figure 10. Simulated spectral efficiency of: blackbody source without any spectral control, ten-layer Si/SiO_2 PhC with blacbody emitter, and ten-layer Si/SiO_2 PhC with 2D tungsten emitter.

PhC's can be designed to selectively radiate due to the combined effect of geometric periodicity and frequency dependant material permittivity. It was shown in Reference 9 that a 2D PhC can drastically alter the radiation pattern of spontaneous emission. Furthermore, the existence of a photonic bandgap enhances the coupling of internal radiation to free-space modes since in the bandgap region there are no guided modes.[9]

Therefore, we have chosen to explore the potential of a 2D hexagonal pattern of air holes in a tungsten substrate for selective emitter applications since it exhibits a complete bandgap (for both TE and TM modes). The existence of a complete bandgap enhances the thermal emission extraction in the low wavelength range. The periodicity of the 2D PhC was chosen to be $a = 1$ μm with a hole diameter of $d = 0.8$ μm. The high-reflectivity of tungsten in the longer wavelength range suppresses thermal emission from the PhC in that wavelength range, while the relatively high-absorption (and equivalently high emittance) of tungsten below 1.8 μm is enhanced by the PhC. Simulation results for the normal emittance of a tungsten 2D PhC shows that at wavelengths shorter than 1.8 μm, emission is significantly enhanced (compared to planar tungsten), while at longer wavelengths it approaches the emittance of planar tungsten (high-reflectance region). The 2D PhC was simulated using Ansoft's HFSS full-wave finite element method (FEM) field solver. The material parameters of tungsten that were used in the simulations can be found in Ref. 10.

4.1. Fabrication of 2D Photonic Crystal

It was decided to carry out the initial fabrication of the 2D structure on a bulk Si substrate and then sputter a layer of tungsten to form the surface coating rather than fabricating directly on a tungsten substrate. The PhC's pattern was defined using interference litography and the holes produced using a reactive ion etch (RIE) technique. Fig. 8 shows a SEM image of a partially etched sample with SiO_2 and chromium mask layers. The sputtering of a layer of tungsten will constitute the final step in the fabrication process. Once this fabrication technique is perfected, a 2D PhC will be fabricated directly on a tungsten substrate. This will allow for high temperature emittance testing to be carried out.

5. CONCLUSIONS AND FUTURE WORK

The analysis presented in this paper highlights how a TPV system with a 2D tungsten PhC emitter and a Si/SiO_2 1D PhC serving as a front side filter exhibits superior performance in terms of efficiency, power density and spectral efficiency, when compared to a TPV system utilizing only a front side filter, as shown in Fig. 9 and Fig. 10. Indeed, the predicted spectral efficiency of this system approaches 90% at 1500K which is twice the spectral efficiency of the TPV system without the 2D emitter. However, these predictions for the performance of the 2D PhC are based on a model which does not take angular effects into account. Fortunately the average hemispherical emittance is not significantly smaller than the normal emittance, and so the results presented above offer a clear motivation for the further study of the potential 1D and 2D PhCs possess in terms of efficiency benefits within TPV systems.

ACKNOWLEDGMENTS

This work was sponsored by MIT/Industry Consortium on Advanced Automotive Electrical/Electronic Components and Systems.

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