International Journal of Energy, Information and Communications
Vol.5, Issue 1 (2014), pp.9-20
http://dx.doi.org/10.14257/ijeic.2014.5.1.02

One-Dimensional Multilayer Microstructure Emitter for Thermophotovoltaic Applications

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Abstract

In this paper, a one-dimensional periodic multilayer is optimized for potential application as thermophotovoltaic (TPV) emitter. The proposed structure was prepared through a magnetron sputtering process. The influence of layers geometric parameters of the proposed structure on the spectral emittance is studied by using the rigorous coupled-wave analysis (RCWA).The emittance spectrum shows three close to unity emission peaks which are explained by the surface plasmon polaritons (SPPs), gap plasmon polaritons (GPPs) and magnetic polaritons (MPs) excitation. The results show that the geometric parameters are very sensitive and important parameter in the emitter fabrication. The normal emittance of the proposed structure is shown to be wavelength-selective and direction-insensitive. The proposed structure can be used as wavelength selective emitter with excellent performance in thermophotovoltaic systems.

Keywords: *Thermophotovoltaic, Multilayer, Rigorous coupled wav analysis (RCWA), Surface plasmon polaritons, Gap plasmon polaritons, Magnetic polaritons*

1. Introduction

Thermophotovoltaic (TPV) devices can convert 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 and solar harvesting energy as well as increasing the conversion efficiency [1-3]. The key components of a TPV system are the thermal emitter that emits radiation and a TPV cell that can generate photocurrent by creating electron-hole pairs. Thermophotovoltaic devices are also a very clean and quiet source of electrical power, portable, reliable and they need almost no maintenance. However, the most obvious drawbacks of TPV devices are their low throughput and poor conversion efficiency, due to the absence of suitable emitters and TPV cells [4]. A TPV device uses an emitter, which is heated up by various energy sources to high temperatures, as a source of radiation for photovoltaic energy conversion. That means a large amount of unusable electromagnetic radiation impinges on the photovoltaic cell (PV) [2, 5]. So, the enhancement of TPV efficiency can be achieved by using selective emitters which are characterized by strong emission at certain wavelengths [5]. The development of selective emitters is very important for energy conversion and photonic systems, such as thermophotovoltaic (TPV) [6-7], solar cells [8- 9] and photodetectors [10]. The emitter temperature in a TPV system generally

ISSN: 2093-9655 IJEIC

ranges between 1000 and 2000K. According to Wien's displacement law, this is optimum to PV cell with a band gap between 0.5 and 0.75 eV. If we take as an example GaSb, which has a low- direct band gap energy about 0.7 eV, the optimum emitter temperature is about 1600K, 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 [3, 11]. An ideal emitter should have high emissivity, close to unity, at short wavelength and low emissivity at long wavelengths. The PV cell absorbs the photons having energies greater than the PV cell band gap, E_g, to generate electron-hole pairs. The photons with energy less than the band gap of TPV cells will result in a destructive heat load on the system components, which will lower the conversion efficiency of the system [1, 12]. A highly efficient TPV device demands the optimization of the output power and throughput. The output power can be increased by using micro/nanostructures in the emitter and filter. This reduces the amount of unusable radiation. The throughput can also be increased by using micro/nanostructures, because it reduces the distance between the emitter and the TPV cell to sub-wavelength dimensions [13-14]. Recently, near-field thermal radiation has been proposed to enhance the throughput and conversion efficiency of TPV by bringing the emitter and TPV cell in close proximity, while the conversion efficiency can be improved by controlling the emission spectrum and directions [1, 15]. Periodic micro/nanostructures in one, two or three dimensional (1D, 2D, or 3D) can enhance the conversion efficiency through the modification of the radiative properties of the electromagnetic waves and thermal emission spectrum [16-17]. A number of micro/nanostructures have been studied to improve the performance of TPV emitters by utilizing different physical mechanisms, such as one-dimensional (1D) deep gratings and 1D complex. These gratings can enhance the emission via excitation of surface plasmon polaritons (SPPs) [16, 18]. 2D microcavities can enhance the emission via cavity resonance (CR) modes [19]. A 3D tungsten photonic crystal [20] and 3D metallic woodpile as a thermophotovoltaic emitter were recently fabricated with the efficiency over 32% [7]. Multilayer microstructures have also been proposed to control thermal radiation [21]. 1D periodic microstructure as TPV emitter was rarely found due to its directionally independent radiative properties. However, the advantage of the 1D periodic microstructures emitter is that it is easy to fabricate with relatively little cost [1, 22]. In this study, we proposed a periodic, 1D microstructure multilayer. The influence of the geometrical parameters on the spectral emittance is studied by using the rigorous coupled wave analysis (RCWA) method [23]. The results can be used to fabricate 1D periodic multilayer microstructures emitter for TPV applications.

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 [24]. 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 [23]. 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. The emittance is calculated from the reflectance according to Kirchhoff's law. Any linearlypolarized incidence can be decomposed into the transverse electric (TE) and transverse magnetic (TM) mode. The normalized electric field of incidence E_{inc} can be expressed as:

$$E_{\text{inc}} = \exp\left(ik_x x + ik_z z - iwt\right) \tag{1}$$

The electric field in region I (Fig. 1a) is the superposition of the incident wave and the reflected waves; therefore

$$E_I\left(x,z\right) = \exp\left(ik_x x + ik_z z\right) + \sum_j E_{rj} \exp\left(ik_{xj} x - ik_{zj}^r z\right) \tag{2}$$

Similarly, the electric field in region IV (E_{IV}) is the a superposition of all transmitted waves

$$E_{IV}\left(x,z\right) = \sum_j E_{tj} \exp\left(ik_{xj} x - ik_{zj}^t z\right) \tag{3}$$

The magnetic field H in region I and IV can be obtained from Maxwell's equation

$$H_I\left(x,z\right) = -\frac{i}{\omega\mu_0}\left(\nabla \times E_I\right) \tag{4}$$

$$H_{IV}\left(x,z\right) = -\frac{i}{\omega\mu_0}\left(\nabla \times E_{IV}\right) \tag{5}$$

where ω represents the frequency and μ_O the magnetic permeability of vacuum. The electric and magnetic field components in region M (Fig1a) can be expressed as a Fourier series:

$$E_M\left(x,z\right) = \sum_j \chi_{yj}\left(z\right) \exp\left(ik_{xj} x\right) y \tag{6}$$

$$H_M\left(x,z\right) = \frac{ik}{\omega\mu_0} \sum_j \left[\gamma_{xj}\left(z\right) x + \gamma_{zj}\left(z\right) z\right] \exp\left(ik_{xj} x\right) \tag{7}$$

Where χ_{yj} and γ_{xj} are vector components for the jth space-harmonic electric and magnetic field in region M (multilayer region), respectively. ε_0 is the electric permittivity in vacuum. Due to the structure periodicity, the relative dielectric function in region M, $\varepsilon(x)$ and its inverse, $1/\varepsilon(x)$ can also be expanded in Fourier series:

$$\varepsilon\left(x\right) = \sum_p \varepsilon_p^{ord} \exp\left(i \frac{2p\pi}{\Lambda} x\right) \tag{8}$$

$$\frac{1}{\varepsilon\left(x\right)} = \sum_p \varepsilon_p^{inv} \exp\left(i \frac{2p\pi}{\Lambda} x\right) \tag{9}$$

Where $\varepsilon_{\text{p}}^{\text{ord}}$ and $\varepsilon_{\text{p}}^{\text{inv}}$ are the jth Fourier coefficient for the ordinary and inverse of $\varepsilon\left(x\right)$, respectively.

3. Proposed Structure

The proposed structure consists of four layers atop a substrate and the image of the scanning electron microscope (SEM) as shown in Figure 1. The layers made of tungsten and silicon dioxide. The geometric parameters used to illustrate a wavelength selective TPV emitter are the thickness of the layers $d_1 = h_1 = 0.06\mu m$, $d_2 = 0.02\mu m$, $h_2 = 0.4\mu m$ and the entire structure is deposited on an opaque tungsten film. Tungsten is usually selected as the emitter material due to its high melting point, good corrosion resistance and its ability to withstand high temperatures [1, 16]. Tungsten emitters have relatively low emissivity in the mid- and far-infrared [25]. They oxidize rapidly in an oxidizing atmosphere at high temperatures. This requires that the emitters must be situated in an inert gas atmosphere or vacuum [26]. The wavelength-dependent dielectric optical constants of tungsten and silicon dioxide, in this work, are obtained from Ref [27].

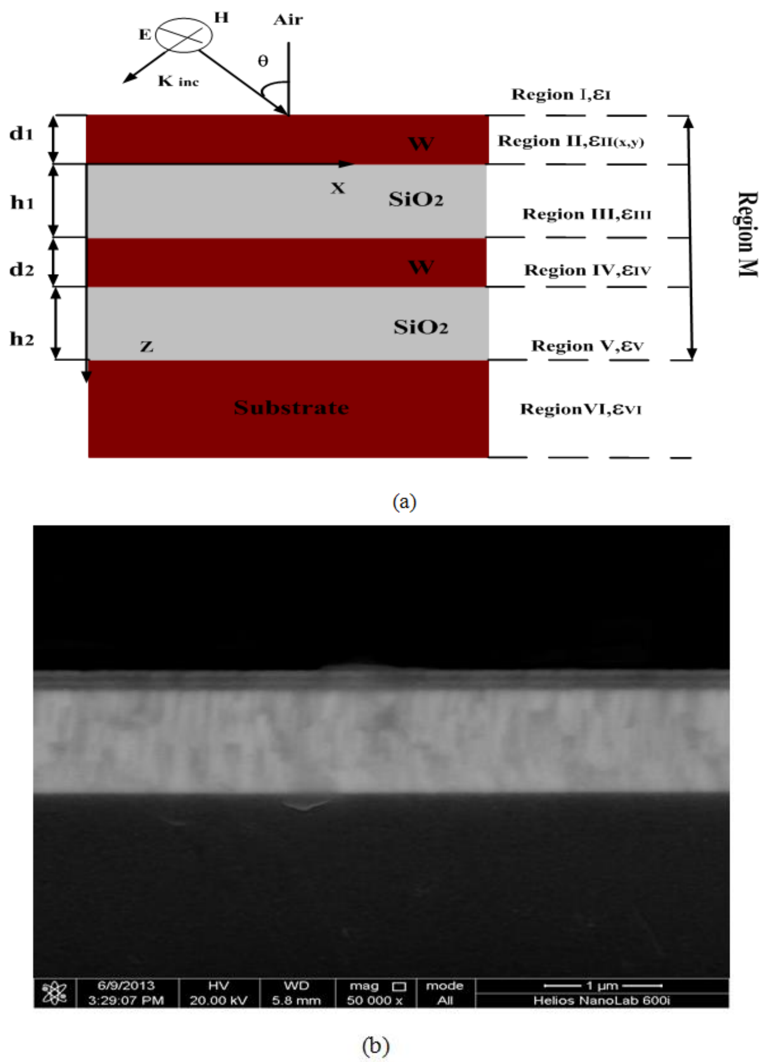


Figure 1. (a)Schematic of the proposed a TPV emitter made of multilayer tungsten and silicon dioxide (b) The image of the SEM

4. Results and Discussion

Figure 2 shows the comparison simulation results on the normal emittance spectrum between the proposed TPV emitter (0.06-0.06- 0.02 - 0.4) μm and the structure that has two layers (0.06-0.06) μm for TM wave. For the proposed structure TPV emitter, the normal emittance spectrum exhibits high value (dashed line □ 0.8) in the spectral range of $0.69<\lambda<1.97\mu m$. The emittance drops below 0.2 at wavelengths above 3.06 μm .Three peaks (>0.9) on the emittance occur in the spectral range of $0.69<\lambda<1.97\mu m$ .The first emission peak at wavelength 0.8 μm occurs due to excitation of the surface plasmon polaritons (SPPs) at the air-tungsten interface, which is confirmed by its polariton dispersion curves those depends on the relative permittivity or dielectric function (*i.e.*, optical constants). The second peak at $\lambda=1.13$ μm occurs due to the interband absorption in tungsten. The (W-SiO_2-W) waveguide can support the propagation of the gap plasmon polaritons (GPPs) mode. The third peak at $\lambda=1.76$ μm is attributed to the excitation of magnetic polaritons (MPs). The excitation of the MPs mode can strongly localize the electromagnetic energy into the dielectric layer which inserted between the top tungsten layer and tungsten substrate. Furthermore, the GPPs mode due to the W-SiO_2-W waveguide is just like placing icing on the cake. The results shown the number of layers is very important parameter to result high emittance value for TPV emitter.

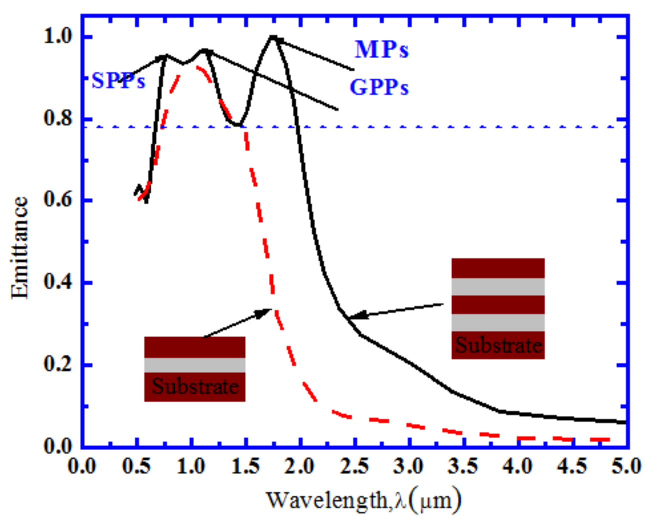


Figure 2. Normal emittance of different TPV emitters for TM waves

4.1 The Effect of Metallic /Dielectric Thickness

The effect of the metallic/dielectric thickness layer on the normal emittance of the proposed TPV emitter is investigated at different thickness of layers. The effect of the metallic layer thickness d_1 on the normal emittance shows in Figure 3 (a). The results shown that the first and second peak moves toward high wavelengths and there is hardly any change in the third peak when the metallic layer thickness d_1 is increased .Two emittance peaks can be seen in Figure 3 (b) when the metallic layer thickness d_2 is bigger than 0.02 μm . The first is attributed to the excitation of (SPPs) and the second one matches the coupling effect of (GPPs) excitation and (MPs) excitation. The high emittance value decreases as the dielectric layer thickness d_2 increases, but the widest bandwidth lies at about $d_2 = 0.02\mu m$ .The results indicates the metallic layer thickness d_2 independence.

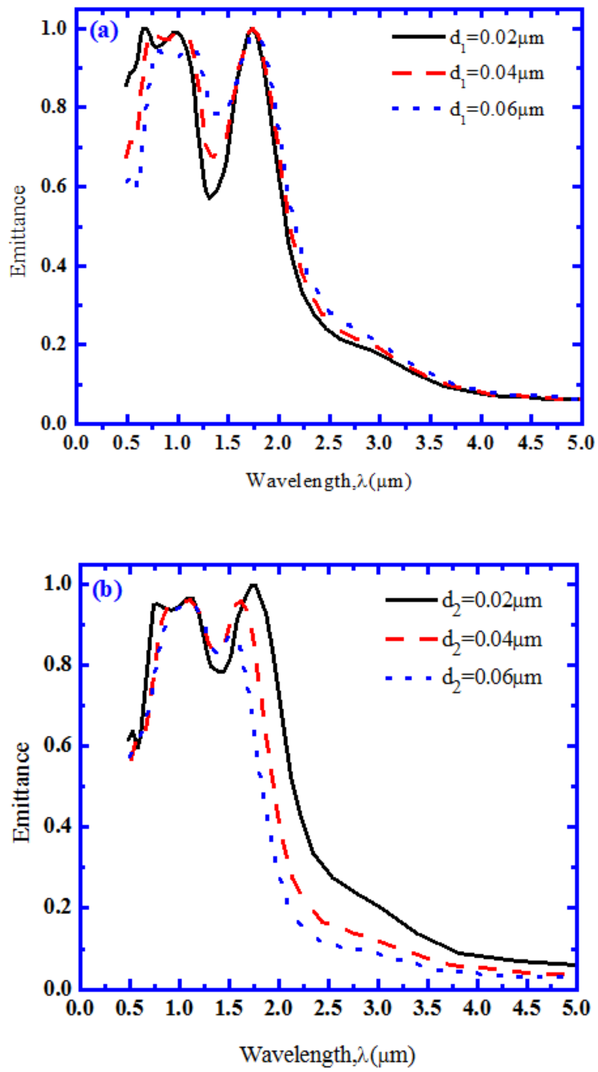


Figure 3. Normal emittance with different (a) d_1 thickness (b) d_2 thickness, for TM waves

The effect of the dielectric layer thickness h_1 on the emittance is shown in Figure 4(a). The results show when the dielectric layer thickness h_1 is increased the first emittance peak decrease and shifts to longer wavelengths while there is hardly any change in the second and the third emittance peak. The results show the dielectric layer thickness h_1 hardly affects the location the second and third peak, but it influences the maximum emittance value for the first peak. In our area of interest, we notice the widest bandwidth lies at about $h_1 = 0.06\mu m$. The dependence of the emittance on the dielectric layer thickness h_2 is shown in Figure4 (b). The results show when the dielectric layer thickness h_2 is increased the third emittance peak shifts to longer wavelengths and also the cutoff wavelength is increased. Of interest is a broad peak, with high emittance, nearly unity, at $h_2 = 0.06\mu m$. The results indicate the independence on the dielectric layer thickness h_2, it also very sensitive and important parameter in the emitter fabrication.

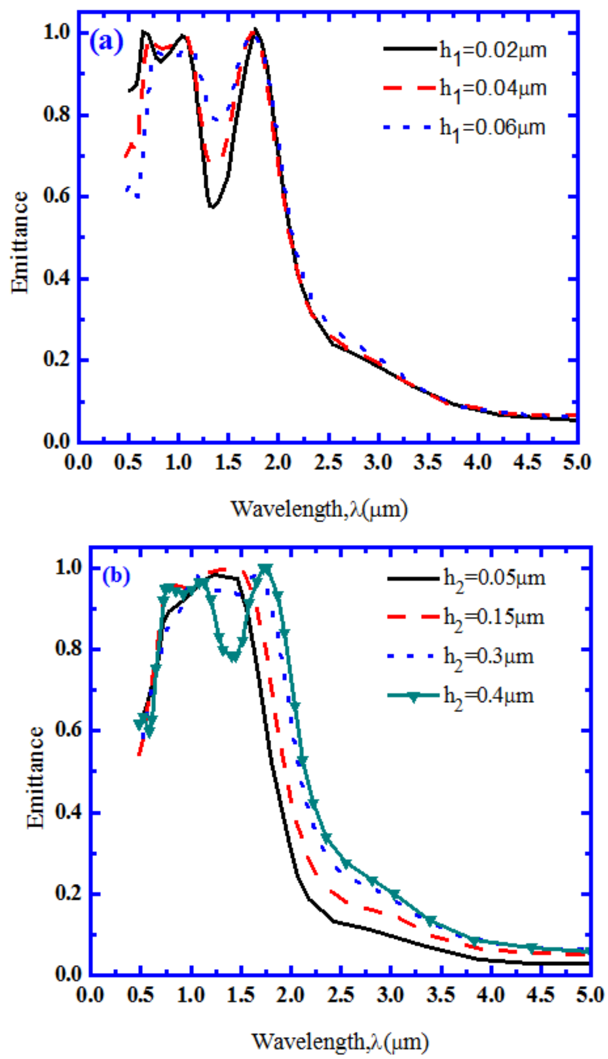


Figure 4. Normal emittance with different (a) h_1 thickness (b) h_2 thickness, for TM waves

4.2 The Effect of Diffraction Orders

The directional-hemispherical reflectance and transmittance can be obtained by summing up the diffraction efficiencies for all orders. All the transmitted energy is absorbed by the tungsten substrate and the emittance can be obtained as according to Kirchhoff's law $(\varepsilon = 1\text{-R})$ where R the reflectance for given wavelength, incidence angle, and polarization. When light impinges onto the multilayer structure, it diffracts into different directions, depending on the wavelength and the layer period. The accuracy of the solution computed for emittance depends solely upon the number of the diffraction orders. The effect of the diffraction orders on the normal emittance of the proposed TPV emitter is also studied for the TM polarization. The results in Figure 5 show the diffraction orders (M) are hardly change in our interest on the normal emittance. Hence, M = 40 is chosen in this study. The emittance spectrum is shown in Figure 2 matches well with the GaSb p-n junction TPV cell, which has a bandgap around 1.78 μm [1]. As mentioned previously, a higher emittance at $\lambda < \lambda_g$ and lower emittance at $\lambda > \lambda_g$ is desired to improve the conversion efficiency for TPV systems. The effect of emittance at $\lambda < 0.5\mu m$ on the conversion efficiency is much weaker according to Planck's blackbody spectral distribution.

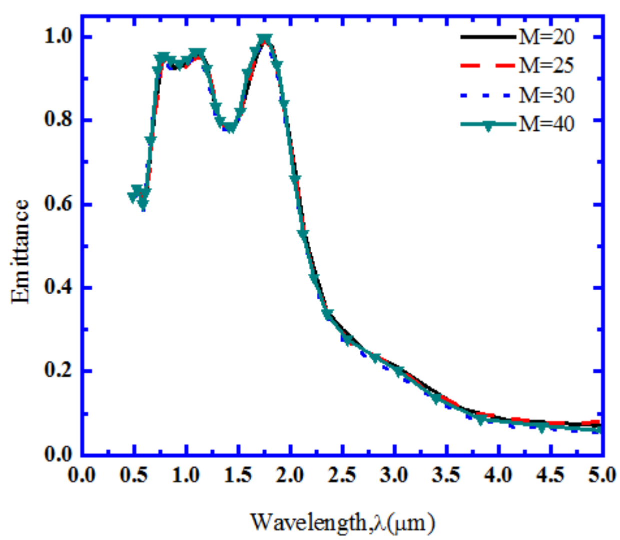
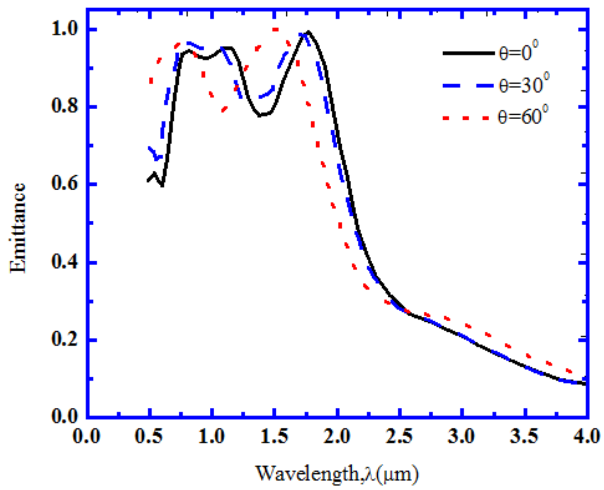


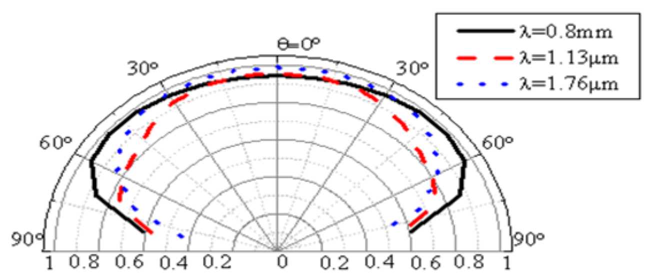
Figure 5. Normal emittance with different diffraction orders for TM waves

4.3 The Effect of the Plane of Incidence

The effect of the plane of incidence (PoI) on the spectral and directional emittance of the proposed TPV emitter is also investigated for different incidence angles at $\lambda = 0.8, 1.13$ and $1.76\mu m$ as shown in Figure 6. The results in Figure 6 (a) show there is hardly any change in the emittance peak when the angle of incidence is increased from 0 to 60^0.The emittance value is higher than 0.9 at $\theta < 45^o$ can be seen in Figure 6(b) for TM waves in the desired wavelength range. It appears that the proposed structure insensitive to direction and it suitable to use as wavelength selective emitter in TPV applications.



(a)



(b)

Figure 6. (a) Spectral emittance (b) The direction emittance, with different incident angles for TM waves

5. Conclusion

The present work has proposed a structure of a TPV emitter consisting of a 1D metallic/dielectric multilayer (tungsten and silicon dioxide). The normal emittance of this proposed structure theoretically is investigated by RCWA method and it is shown to be wavelength selective. The three close to unity emission peaks in spectral emittance of the proposed structure are explained by the mechanisms of the SPPs, GPPs and MPs excitation. The geometrical parametric of the proposed structure, diffraction orders and incident angles are investigated. The results show that emitter performance is very sensitive to the layers thickness but insensitive to direction. This study helps to understand the excitation mechanisms of SPP, GPP, and MP, and also it facilitates future design optimization for practical applications and development of wavelength-selective emitter in thermophotovoltaic systems.

Acknowledgements

This work is supported by the Foundation for Innovative Research Groups of the National Natural Science Foundation of China (No. 51276049) and the Fundamental Research Funds for the Central

Universities (No. HIT. BRETIII.201227). A very special acknowledgement is made to the editors and referees whose constructive criticism has improved this paper.

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