Research Article
One-dimensional Microstructure Tungsten Gratings for Thermo Photovoltaic Applications

[1,3]Samah. G. Babiker, [1]Shuai Yong, [2]Mohamed Osman Sid-Ahmed and [1]Xie Ming
[1]Department of Engineering Thermo Physics-School of Energy Science and Engineering,
Harbin Institute of Technology, Box. 456, 92 West DaZhi Street,
NanGang District, Harbin City, Zip Code: 150001, P.R. China
[2]Sudan University of Science and Technology, Sudan
[3]University of the Holy Quran and Islamic Sciences, Sudan

Abstract: In this study, a one-dimensional microstructure tungsten grating is optimized for potential application as Thermo Photovoltaic (TPV) emitter. The influence of gratings geometric parameters on the spectral emittance are studied by using the Rigorous Coupled-Wave Analysis (RCWA). The results show that the spectral emittance is affected by the gratings geometrical parameters and insensitive to the direction. The optimum parameters of the proposed structure are grating period 1.4 µm, a filling ratio 0.8 and grating height 0.2 µm. A broad peak of high emittance is obtained at wavelengths between 0.5 and 1.8 µm. A peak emittance close to unity at wavelengths between 0.5 and 2 µm is achieved and it drops below 0.2 at wavelengths above 2 µm. This can be explained by the surface plasmon polaritons excitation coupled with the grating microstructures. At longer wavelengths, the emittance remains low and this is highly desired for thermo photovoltaic applications to reduce the thermal leakage due to low-energy photons that do not produce any photocurrent. The proposed structure can be used as a selective emitter for TPV applications.

Keywords: Emittance, grating, Rigorous Coupled-Wave Analysis (RCWA), selective emitter, surface plasmon polaritons, thermo photovoltaic

INTRODUCTION

Thermo Photovoltaic (TPV) devices 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 (Basu *et al*., 2007; Wang and Zhang, 2012; Mostafa *et al*., 2012). The TPV device consists of heat source and optical cavity which comprises of a thermal radiator (emitter), filter and photovoltaic PV cell. Advantages TPV device promises to be a very clean and quiet source of electrical power, portable, good reliability and safe. As a result, TPV device can be more commonly used in many applications such as recycling waste energy from industrial processes, electric-grid independent appliances, military applications and it has a very good potential to be an alternative to traditional (Coutts, 1999; Jovanovic, 2005; Yang *et al*., 2003). The most obvious drawbacks of TPV devices are their low throughput and poor conversion efficiency, due to the absence of suitable emitters and the TPV cells (Coutts *et al*., 2003). A highly efficient TPV device demands

increase to output power and throughput. The output power can be increased by using micro/nanostructures in components of TPV device (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 (Chen, 2007; Whale, 2001). 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) (Wang and Zhang, 2012; Diso *et al*., 2003). So, the enhancement of TPV efficiency can be achieved by using selective emitters which are characterized by strong emission at certain wavelengths (Diso *et al*., 2003). The development of selective emitters is very important for energy conversion and photonic devices, such as Thermo Photovoltaic (TPV) devices (Sai *et al*., 2005a; Nagpal *et al*., 2008), solar cells (Boueke *et al*., 2001; Zhang, 2000) and photo detectors (Sharma *et al*., 2002).

In this study we investigate the spectral emittance of one-dimensional (1D) periodic microstructure

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tungsten (W) gratings. The goal is to manufacture radiation emitters for the Near Infrared (NIR) spectral range, that show a wavelength selective radiative properties based on Surface Plasmon Polariton excitation effects (SPPs).

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 (Chen and Zhang, 2007; Fu and Zhang, 2009). Microstructures such as 1D deep gratings can enhance the emission via excitation of Surface Plasmon Polaritons (SPPs) (Chen and Zhang, 2007; Hesketh *et al*., 1986) and 2D microcavities can enhance the emission via Cavity Resonance (CR) modes (Maruyama *et al*., 2001).

The emitter temperature in a TPV device generally ranges between (1000 and 2000) K according to (Wien's displacement Law) corresponding to an optimum PV cell with a band gap between (0.5-0.75) eV. If we take as an example GaSb, which has a low-direct band gap energy of 0.7 eV, the optimum emitter temperature is about 2000 K, corresponding to a wavelength of 1.78 μm. This makes it a good choice for a TPV device which transfers the photon energy into electricity (Mostafa *et al*., 2012; Jovanovic, 2005). 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 and directly convert into electricity (generate electron-hole pairs) by using photovoltaic effect. 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 (Basu *et al*., 2007; Chia and Feng, 2007).

Recently, several microstructures have been developed to enhance the efficiency of TPV device based on different physical mechanisms. This includes 1D periodic gratings as a TPV emitter was proposed (Wang and Zhang, 2012), 1D complex grating (Chen and Zhang, 2007), 1D Photonic Crystal (PhC) (Narayanaswamy and Chen, 2004). Development of 2D structure includes tungsten gratings emitter with thermally excited Surface Plasmons Polaritons (SPPs) deep micro cavities with cavity resonance modes and tungsten grating experimentally demonstrated a strong emission peak and high thermal stability over 1400 K (Sai *et al*., 2003a; Sai *et al*., 2005b; Sai *et al*., 2003b). A 3D tungsten photonic crystal (Lin *et al*., 2003) and 3D metallic woodpile as a TPV emitter was recently fabricated with an efficiency which exceeds 32% (Nagpal *et al*., 2008). 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 compared with 2D and 3D periodic microstructures emitter (Basu *et al*., 2007; Nguyen-Huu *et al*., 2012). In

this study, we proposed periodic, 1D microstructure tungsten grating. The influence of the geometrical parameters on the spectral emittance is studied by using numerical calculations Rigorous Coupled Wave Analysis (RCWA) method (Moharam and Gaylord, 1981). The results can be used to fabricate 1D periodic microstructures tungsten emitter with micro-cavities.

CALCULATION METHOD

Rigorous Coupled-Wave Analysis (RCWA) method is used for analyzing the diffraction of electromagnetic waves by periodic gratings (Peng and Morris, 1995). It is used in this study to calculate the spectral emittance of the periodically, micro-structured surfaces. RCWA is used to analyze the general grating diffraction problem by solving Maxwell's equations accurately in each of the three regions (input, grating and output) based on a Fourier expansion (Moharam and Gaylord, 1981). 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 material:

$$\varepsilon = (n + ik)^2$$

where,
n = The refractive index
k = 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 angle (θ) is the corresponding emission angle and the emittance is calculated from the reflectance based on Kirchhoff's law. The parameters used to describe 1D microstructures tungsten gratings and the state of incident wave are defined as periodicity (Λ), grating width (w), groove width (a) and grating height (h). Any linearly-polarized incidence can be decomposed into the Transverse Electric (TE) wave and the Transverse Magnetic (TM) wave. The normalized electric field of incidence E_{inc} can be expressed as:

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

The electric field in region I (E_I) is the superposition of the incidence wave and the reflected waves; therefore:

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

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

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

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

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

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

where,
ω = Frequency
μ_0 = The magnetic permeability of vacuum

The electric and magnetic field components in region II can be expressed as a Fourier series:

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

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

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

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

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

where, ε_p^{ord} and ε_p^{inv} are the jth Fourier coefficient for the ordinary and inverse of $\varepsilon(x)$, respectively.

PROPOSED STRUCTURE

The proposed structure consists of grating layer atop a substrate, as shown in Fig. 1 and it is depicted by a period (Λ), width (w), height (h) of the grating, the groove width ($a = \Lambda - w$) and a filling ratio $f = {}^w/_\Lambda$. The grating ridge and supporting substrate are both made of tungsten; tungsten is usually selected as the emitter material due to it has good properties such as, high melting point, good corrosion resistance and can withstand high temperatures (Basu *et al.*, 2007; Chen and Zhang, 2007). Tungsten emitters have relatively low emissivity in the mid- and far-infrared (Sai *et al.*, 2004). 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 (Qiu and Hayden, 2012). The wavelength-dependent dielectric optical constants of tungsten are obtained from Ref (Lunch and Hunter, 1998).

The emitters usually operate at high temperatures and their spectral emittance should be high at wavelengths less than 1.78 µm, where GaSb cell has high quantum efficiency (Bett and Sulima, 2003). The high emittance of 1D microstructure gratings can be generated by either Cavity Resonance (CR) modes (deep grating) or the excitation of Surface Plasmon Polaritons (SPPs) (shallow grating). Since depth increment is difficult in micro fabrication, the SPPs excitation is more appropriate than cavity resonance modes for high emittance generation and the emittance peak is usually sharp. SPPs excitation is a coupled, localized electromagnetic wave that propagates along the interface between two different media, due to charge density oscillations and the EM field can be greatly enhanced near the interface (Raether, 1988). SPPs excitation leads to a strong absorption and a sharp
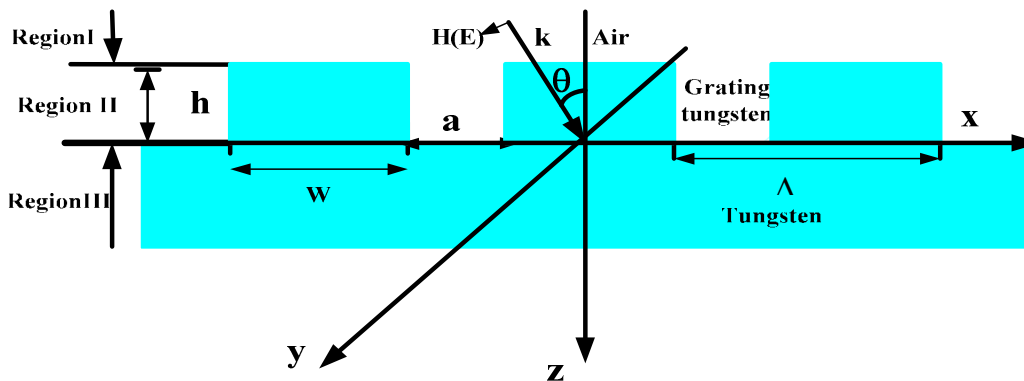

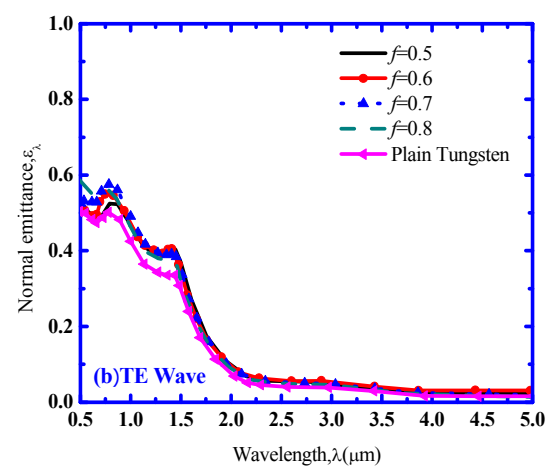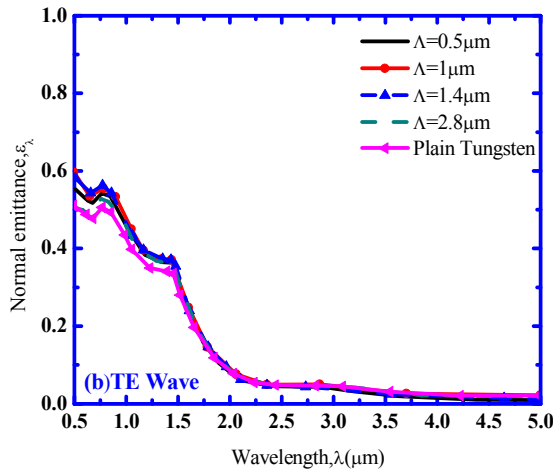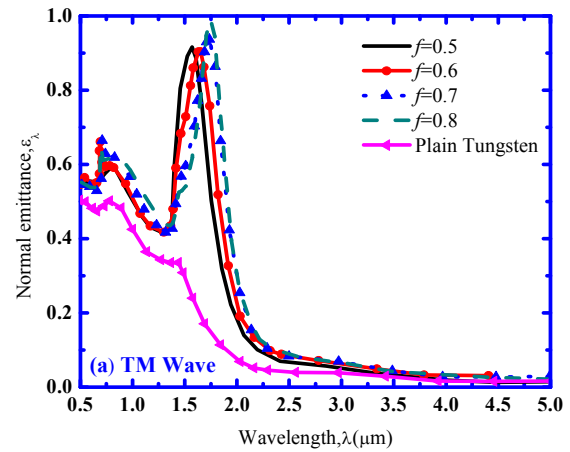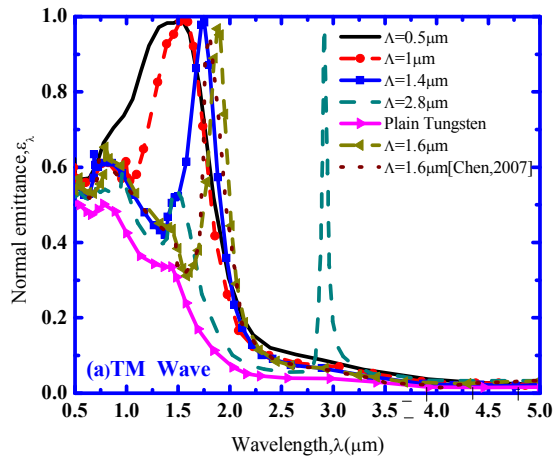Fig. 1: Basic geometry grating 1D microstructure selective emitter

Fig. 2: Normal emittance of plain tungsten and proposed structure for different grating periods, $f = 0.8$ and $h = 0.2$ μm for (a) TM (b) TE wave

Fig. 3: Normal emittance of plain tungsten and proposed structure for different filling ratio, $\Lambda = 1.4$ μm and $h = 0.2$ μm for (a) TM (b) TE wave

reflectance reduction in a limited wavelength range (Park *et al*., 2005). According to Kirchhoff's law, the directional-spectral emittance is the same as the spectral absorptance of surface (Chen and Zhang, 2007; Heinzel *et al*., 2000). The spectral position and the strength of this excitation depend on the grating period, the shape of the grating grooves and the polarization (Sai *et al*., 2003a; Heinzel *et al*., 2000). The requirement of SPP excitation can be met by the incident radiation with a magnetic field component parallel to the grating vector (x-direction). In the present study, two cases with plane of incidence (perpendicular TM and parallel TE) to the grooves of the grating are studied.

RESULTS AND DISCUSSION

Effect of gratings period on the spectral emittance:
The normal emittance spectra of the proposed structure when $h = 0.2$ μm, $f = 0.8$ and different grating periods (Λ) (0.5, 1, 1.4 and 2.8) μm are shown in Fig. 2a for

TM and in Fig. 2b for TE wave. The emittance of a plain tungsten emitter is also shown for comparison. In Fig. 2a, the emittance peak shifts towards longer wavelengths (cutoff wavelength increases) as the grating period increases. The emittance peak much broaden with the $\Lambda = 0.5$ and 1 μm. The emittance is very sharp and close to unity for $\Lambda = 1.4$ at $\lambda = 1.76$ μm. The spectral emittance for $\Lambda = 2.8$ μm is also shown for comparison. The normal emittance of plain tungsten is not high enough at short wavelengths, so it cannot be a suitable for TPV emitters. The results are in agreement with the results shown in Ref (Chen and Zhang, 2007).

Effect of gratings width on the spectral emittance:
The effect of grating width (w) on the spectral emittance is studied with different filling ratio (f) (0.5, 0.6, 0.7 and 0.8), $h = 0.2$ μm and grating period of $\Lambda = 1.4$ μm for TM and TE respectively at normal incidence. The results in Fig. 3 show the filling ratio
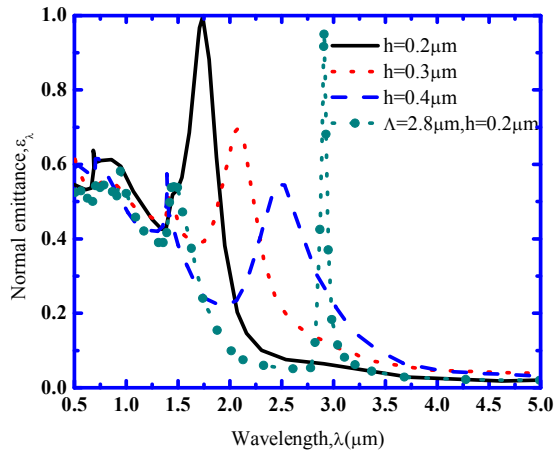
Fig. 4: Normal emittance of the proposed structure with different grating height, Λ = 1.4 μm and f = 0.8 for TM
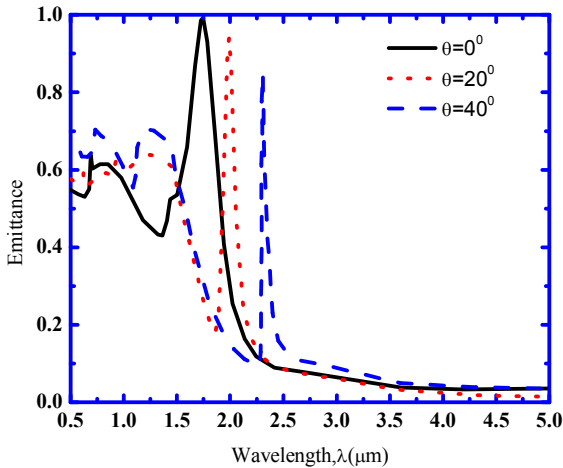

Fig. 5: Spectral emittance of the proposed structure with different incidence angles, Λ = 1.4 μm, h = 0.2 μm and f = 0.8 for TM wave

does not affect the peak location but it influences the maximum value significantly. In our area of interest, we notice a high emittance peak close to unity at λ = 1.76 μm and f = 0.8. It has to be noticed that the filling ratio is proportional to the grating width.

Effect of gratings height on the spectral emittance: Figure 4 shows the spectral emittance of the proposed structure with Λ = 1.4 μm, f = 0.8 for different grating heights (h) (0.2, 0.3 and 0.4) μm for TM waves at normal incidence. The results show when the grating height is increased the emittance peaks decrease and shifts to longer wavelengths. The spectral emittance for Λ = 2.8 μm and h = 0.2 μm is also shown for comparison. It should be noticed that the emittance peak is strongly affects by the grating height (h). Of

interest is a sharp peak, with high emittance, close to unity, at h = 0.2 and λ = 1.76 μm.

Effect of the plane of incidence on the spectral emittance: The effect of the Plane of Incidence (POI) on the spectral emittance of the proposed structure is shown in Fig. 5. When incidence angle increases the emittance peak becomes very sharp, the cutoff wavelength increases.

The proposed structure for selective emitters depends on the kind of PV cells which used in the system. For this study, we selected GaSb as the PV cell because it is has a low energy direct band gap (E_g 0.7eV) and easy fabrication using commercial fabrication processes (Mostafa *et al*., 2012; Jovanovic, 2005). The sensitive region of GaSb cell is about 0.6 to 1.8 μm. From the simulated results, we choose Λ = 1.4 μm, f = 0.8 and h = 0.2 μm as the optimum parameters to fabricate selective emitters.

CONCLUSION

The present study we have studied a structure consisting of 1D microstructure tungsten (gratings), for design and development of a spectrally selective emitters that are to be used in TPV applications. The effect of geometric parameters on the spectral emittance is investigated by Rigorous Coupled-Wave Analysis (RCWA) method. The emittance peak value of the proposed structure is close to unity with a grating period Λ = 1.4 μm, a filling ratio f = 0.8 and grating height h = 0.2 μm at emitter temperature about 1600K at λ = 1.76 μm but it is lower than 0.2 at λ>2.09 μm. The proposed structure can be applied to fabricate selective emitters for TPV applications.

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