# Design of One – Dimensional Tungsten Gratings for Thermophotovoltaic Emitters

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*Abstract*—In this paper, a one - dimensional microstructure tungsten grating (pyramids) is optimized for potential application as thermophotovoltaic (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. The optimum parameters are grating period of 0.5µm, a filling ratio of 0.8 and grating height of $h$=0.2µm. A broad peak of high emittance is obtained at wavelengths between 0.5 and 1.8µm. The emittance drops below 0.2 at wavelengths above 1.8µm. 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 thermophotovoltaic 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 a narrow band gap cell such as GaSb. The performance of this simple 1-D emitter proved to be superior to that from more complicated structures. Almost all the radiation from the emitter incident, at angles up to 40°, on the cell, could be utilized to produce a photocurrent. There is no need for a filter.

*Keywords*—Thermophotovoltaic, RCWA, Grating, Emittance, Surface plasmon polaritons.

## I. INTRODUCTION

THERMOPHOTOVOLTAIC (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 [1]-[3]. 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 [4]. 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

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reduces the distance between the emitter and the TPV cell to sub-wavelength dimensions [5], [6]. 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], [7]. So, the enhancement of TPV efficiency can be achieved by using selective emitters which are characterized by strong emission at certain wavelengths [7]. The development of selective emitters is very important for energy conversion and photonic devices, such as thermophotovoltaic (TPV) devices [8], [9], solar cells [10], [11] and photodetectors [12].

In this paper we investigate the spectral emittance of a one – dimensional (1D) periodic microstructure tungsten grating (pyramids). The goal is to manufacture radiation emitters for the near infrared (NIR) spectral range, that show 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 [13], [14]. Microstructures such as 1D deep gratings can enhance the emission via excitation of surface plasmon polaritons (SPPs) [13], [15], and 2D microcavities can enhance the emission via cavity resonance (CR) modes [16].

The emitter temperature in a TPV system generally 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 0.75eV. If we take as an example GaSb, which has a low- direct band gap energy of 0.72eV, the optimum emitter temperature is about 2000K, corresponding to a wavelength of 1.73µm. This makes it a good choice for a TPV system which transfers the photon energy into electricity [3], [17]. 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], [18].

Recently, several microstructures have been developed to enhance the efficiency of TPV device based on different physical mechanisms. This includes 1D periodic gratings, 1D complex grating and 1D photonic crystal (PC), made of tungsten and alumina [2], [13], [19]. While 1D periodic microstructures refers to either vertically layered structures or laterally-structured surfaces. Development of 2D structure

includes tungsten gratings emitter with thermally excited surface plasmons polaritons (SPPs), deep microcavities with cavity resonance modes and tungsten grating. This has experimentally demonstrated a strong emission peak and high thermal stability over 1400K [20]-[22]. A 3D tungsten photonic crystal and 3D metallic woodpile emitter were recently fabricated with an efficiency which exceeds 32% [9], [23].

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], [24].

In this study, we proposed 1D periodic microstructures tungsten pyramidal gratings. The influence of the geometrical parameters on the spectral emittance is studied by using the rigorous coupled wave analysis (RCWA) method [25]. The results can be used to fabricate 1D periodic microstructures tungsten emitter with micro-cavities.

## II. 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 [26]. 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, grating, and output), based on Fourier expansion [25]. 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. The parameters used to describe 1D microstructures tungsten gratings and the state of incident wave are defined as periodicity $(\Lambda)$, grating width $(w)$, groove width $(a)$, grating height $(h)$ and incident angle $(\theta)$. Any linearly-polarized 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:

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

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

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

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

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

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

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

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

where $\omega$ represents the frequency and $\mu_0$ the magnetic permeability of vacuum. The electric and magnetic field components in region II can be expressed as a Fourier series:

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

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

where $\chi_{yj}$ and $\gamma_{xj}$ are vector components for the jth space-harmonic electric and magnetic field in region II (grating region), respectively. $\varepsilon_0$ is the electric permittivity in vacuum. Due to the structure periodicity, the relative dielectric function in region II, $\varepsilon(x)$ and its inverse, $\dfrac{1}{\varepsilon(x)}$, can also be expanded in Fourier series:

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

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

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

## III. PROPOSED STRUCTURE

The proposed structure consists of a grating layer (pyramids) atop a substrate, as shown in Fig. 1. It is depicted by a period $(\Lambda)$, width $(w)$, height of the grating $(h)$, 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 its high melting point, good corrosion resistance and its ability to withstand high temperatures [1], [13]. Tungsten emitters have relatively low emissivity in the mid- and far-infrared [27]. 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 [28]. The wavelength-dependent dielectric optical constants of tungsten, in this work, are obtained from [29].

If the emitter is to be used with GaSb PV cell, its spectral emittance must be high at wavelengths less than $1.73\mu m$, to give maximum efficiency for the cell [30]. The high emittance of 1D microstructure gratings can be generated by either cavity resonance modes (deep grating) or the excitation of surface plasmon polaritons (SPPs) (shallow grating). Since depth increment is difficult in microfabrication, the surface plasmon polaritons (SPPs) excitation is more appropriate. SPPs excitation is a coupled, localized electromagnetic wave that propagates along the interface between two different media, due to charge density oscillations. The electromagnetic field can be greatly enhanced near the interface [31]. SPPs excitation leads to a strong absorption and a sharp reflectance reduction in a limited wavelength range [32]. According to Kirchhoff's law, the directional-spectral emittance is the same as the spectral absorptance of surface [13], [33]. The spectral position and the strength of this excitation depend on the grating period, the shape of the grating grooves and the polarization [20], [33].

The requirement of SPP excitation can be met by incident radiation with a magnetic field component parallel to the grating vector (x-direction). In the present work two cases, with perpendicular TM and parallel TE to the grooves of the grating, are studied.
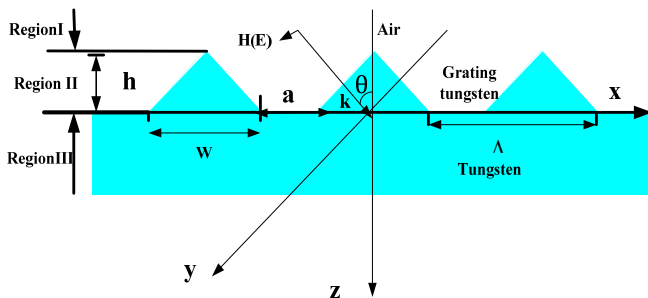


Fig. 1 Basic geometry the grating of a 1D microstructure selective emitter

## IV. RESULTS AND DISCUSSION

### A. Effect of Gratings Period

The emittance spectra, when $h = 0.2\mu m$, $f = 0.8$ and different grating periods $(\Lambda)$ (0.5, 1, 1.5 and 3) $\mu m$, are shown in Fig. 2 (a) for TM perpendicular to the grooves and in Fig. 2 (b) for TE parallel to the grooves, for a wave at normal incidence. The emittance of a plain tungsten emitter is shown for comparison. In Fig. 2 (a), the emittance peak shifts towards longer wavelengths as the grating period increases. The emittance is close to unity for the grating period $\Lambda = 0.5$. The peak is at wavelength 1.51 μm. The results are in agreement with the results shown in [13].
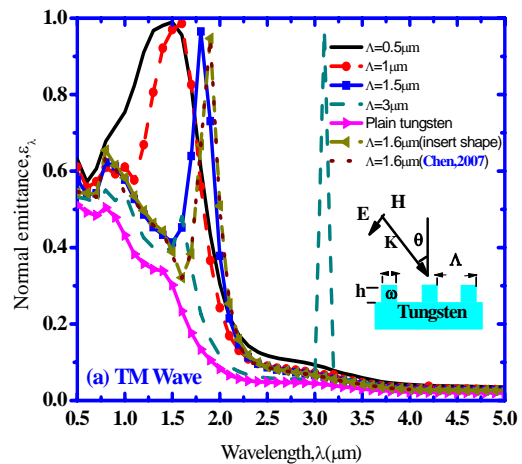


Fig. 2 (a) (Color online) Normal emittance with different grating period, $f = 0.8$ and $h = 0.2\mu m$, when TM is perpendicular to the grooves
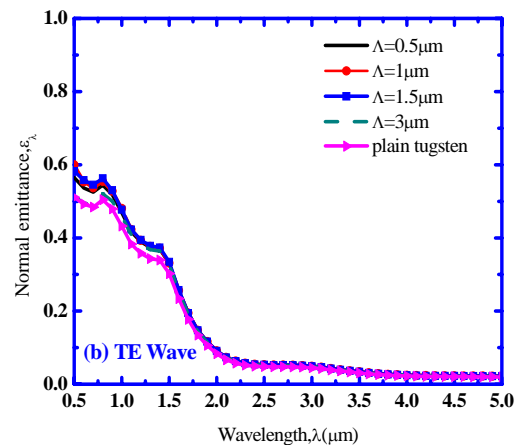


Fig. 2 (b) (Color online) Normal emittance of plain tungsten and proposed structure with different grating period, $f = 0.8$ and $h = 0.2\mu m$, when TE is parallel to the grooves

*B. Effect of Gratings Width*

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), $h = 0.2 \mu m$ and grating period of 0.5µm, for TM perpendicular and TE parallel to the grooves, at normal incidence. The results in Fig. 3 show the filling ratio hardly affects the peak location, but it influences the maximum emittance value. In our area of interest, we notice a high emittance peak (nearly unity) at wavelength 1.51µm and $f = 0.8$. It has to be noticed that the filling ratio is proportional to the grating width.
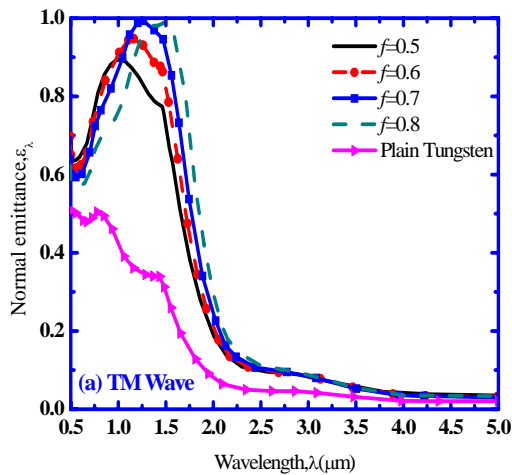


Fig. 3 (a) (Color online) Normal emittance for different filling ratio, $\Lambda = 0.5 \mu m$ and $h = 0.2 \mu m$, when TM is perpendicular to the grooves
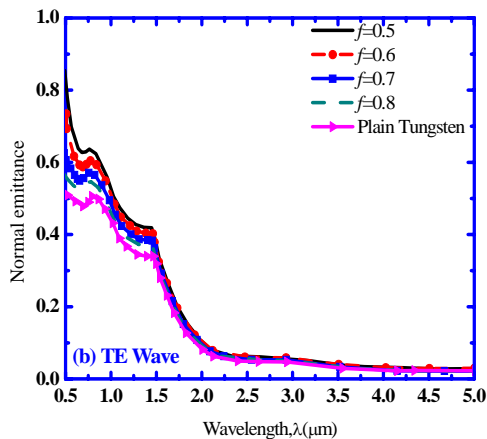


Fig. 3 (b) (Color online) Normal emittance for different filling ratio, $\Lambda = 0.5 \mu m$ and $h = 0.2 \mu m$, when TE is parallel to the grooves

*C. Effect of Gratings Height*

Fig. 4 shows the spectral emittance of the proposed structure with grating period of 0.5 and $f = 0.8$, for different grating height $(h)$ (0.2, 0.3 and 0.4) $\mu m$, at normal incidence angle. The results show when the grating height is increased the emittance peaks decrease and shifts to longer wavelengths. Of interest is a broad peak, with high emittance, nearly unity, at h = 0.2 and wavelength about 1.51µm. The cutoff wavelength is about 2.2µm.
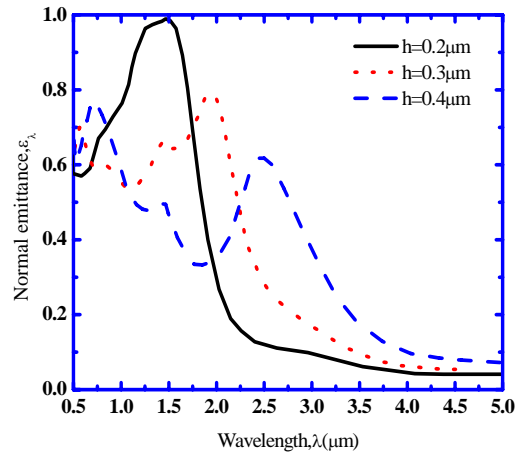


Fig. 4 (Color online) Normal emittance with different grating height, $\Lambda = 0.5 \mu m$ and $f = 0.8$, when TM is perpendicular to the grooves

*D. Effect of the Plane of Incidence*

The effect of the plane of incidence on the spectral emittance is shown in Fig. 5. There is hardly any change in the emittance when the angle of incidence is increased from 0 to $40^0$. It appears that this simple 1-D structure satisfies the requirements for a TPV system. The results are even better than that from the complex grating of [13].
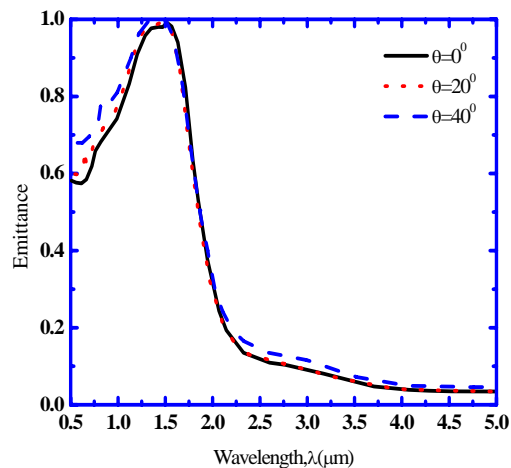


Fig. 5 (Color online) Spectral emittance with different incidence angles, $\Lambda = 0.5 \mu m$, $h = 0.2 \mu m$ and $f = 0.8$ for TM wave

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 $\left( E_g \simeq 0.7 eV \right)$ and easy fabrication, using commercial fabrication processes. The sensitive region of GaSb cell is about 0.6 to 1. 8 $\mu m$ .From the simulated results, we choose a grating period of 0.5µm, $f = 0.8$ and $h = 0.2 \mu m$ as the optimum parameters to fabricate selective emitters

## V. Conclusion

The present work, we have studied a 1D tungsten microstructure (pyramid gratings), for design and development of a spectrally selective emitters that are to be used in TPV applications. The effect of the 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 of 0.5 µm, a filling ratio of 0.8 and a grating height of $h = 0.2 \mu m$ , at emitter temperature of about 1900K. The emitter has a broad peak at short wavelengths and a cutoff wavelength of about 2.2µm. This is at all angles of incidence up to $40^0$. The emitter is found to satisfy the optimum quantum efficiency of a GaSb cell. There is no need for a filter. Almost all the radiation from the emitter would be converted to a photocurrent. The simple 1-D structure proved to be superior to more complicated structures.

## Acknowledgment

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