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Tungsten Complex Gratings as a Thermophotovoltaics Selective Emitter

Samah G .Babiker[1, 2], Mohamed O. Sid-Ahmed[3], Yong Shuai[4] and Ming Xie[4]

[1]*Department of Physics -Faculty of medicine-University of Dammam - Kingdom of Saudi Arabia*

[2]*Department of Physics -Faculty of Education-University of the Holy Quran and Islamic Sciences-Omdurman-Sudan*

[3]*Department of Physics - Faculty of Sciences- Sudan University of Science and Technology, Khartoum-Sudan*

[4]*Department of Engineering Thermophysics-School of Energy Science and Engineering Harbin Institute of Technology- Harbin - P.R. China*

samahgas@yahoo.com

Abstract

A kind of concave tungsten complex grating based on superposition of two simple binary tungsten gratings with different groove depths has been proposed for potential application as thermophotovoltaic (TPV) selective emitters. The effect of the simple grating geometric parameters on the spectral emittance is calculated numerically by using the rigorous coupled-wave analysis (RCWA). The emittance of the complex grating shows broadband-directional insensitive peak in the spectral region where the quantum efficiency of TPV cells is high, which is explained by the surface plasmon polariton (SPP). The results show that the complex grating has high emittance value, above 0.8, within the spectral range of 0.8 $\mu m \le \lambda \le 1.76 \mu m$ *. 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. It is concluded that the complex grating has great potential to be used as a selective emitter for TPV applications.*

Keywords: *Thermophotovoltaic, Selective emitter, Tungsten, Complex gratings, Rigorous coupled wave analysis (RCWA), surface plasmon polariton (SPP)*

1. Introduction

Development of wavelength-selective absorbers and emitters has been widely studied for various energy conversion systems, such as solar cells [1] and thermophotovoltaic (TPV) devices. 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 electromagnetic waves [3-4] and thermal emission spectrum.

Periodic gratings can also excite surface electromagnetic (EM) waves, or polaritons, resulting in coherent thermal emission [5]. One dimensional (1D) deep gratings [6] and 2D microcavities [7] can enhance the emission via resonance modes.

The emitter temperature in a TPV system generally ranges between 1000 and 2000 K, corresponding to the wavelengths required by low band gap cells, such as GaSb cell, which is typically used in TPV systems to transfer the infrared photons energy into electricity. This conversion occurs when the photon energy is higher than the energy corresponding to the bandgap of TPV cells. Photons having energies less than the TPV cell bandgap (sub-band gap photons) would be absorbed beyond the depletion region, and so they cannot produce photocurrent and should be avoided to prevent thermal leakage

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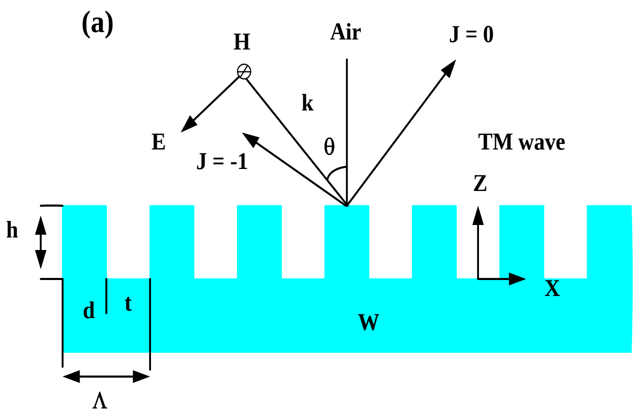
that would reduce the efficiency. An ideal TPV emitter should have high emissivity close to unity corresponding to the spectral region, where a TPV cell has high quantum efficiency and as low as possible outside that region. It also needs to be polarization-insensitive so that high emissivity for both transverse electric wave (TE wave or s-polarization) and transverse magnetic wave (TM wave or p- polarization) can be achieved. Furthermore, the spectral emittance peak of a TPV emitter should be independent of the direction to maximize the efficiency [2].

A number of periodic microstructures have been developed to improve the performance of TPV emitters. Narayanaswamy and Chen [8] analyzed theoretically thermal emission from 1D metallodielectric periodic structures which exhibited enhancement in the emissivity. Heinzel *et al.*, [9] manufactured 2D tungsten gratings and they achieved high emittance in near-infrared spectral range through the thermally excited surface plasmons. Sai *et al.*, [10-12] experimentally demonstrated the potentials of 2D deep periodic tungsten microcavities by applying the cavity resonance modes to obtain higher emittance for TPV emitters. Lin *et al.*, [13] fabricated 3D tungsten photonic crystals with enhanced absorption/emission in the near-infrared region. Multilayer microstructures have also been proposed to control thermal radiation [14]. Recently, Wang and Zhang [15] used a 1D tungsten grating/thin-film nanostructure as a selective TPV emitter which achieved high emittance in the near-infrared spectral range by exciting magnetic polaritons (MPs) and surface plasmon polaritons (SPPs). Chen and Zhang [2] proposed 1D complex grating as a wavelength selective emitter. The emittance was enhanced by surface plasmon polaritons (SPPs). The 1D surface periodic structures are widely employed because, they are easier to fabricate with relatively little cost than the 2D and 3D structures [16-17]. The most obvious disadvantages of 1D structures are their sharpness and angle dependence of the spectral emittance peak. Recently other alternative designs, the complex gratings, have been proposed, which can overcome the disadvantages of 1D grating [18-21]. The complex gratings have shallow groove depth and may be easier to fabricate than 2D and 3D structures. The complex grating is a concept that the grating features are a superposition of two or more 1D simple binary grating with different periods and features. The complex grating which contain the simple gratings have shown broadband, wavelength selective and direction-insensitive high absorptance/emittance in the ultraviolet [19], near- infrared [21] and microwave [20] regions. The complex gratings with different groove depths have been less investigated. Wan [22] investigated the manipulation of thermal emission by using 1D simple tungsten gratings with different groove depths. Cheng *et al.*, [23] proposed concave silicon complex gratings with different groove depths for a potential application as an absorber for solar cells in the visible and near-infrared wavelength regions.

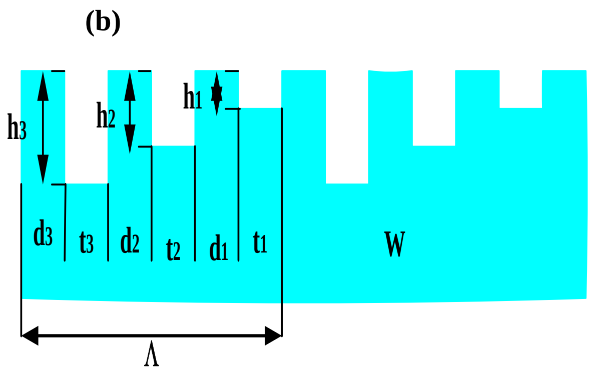
In this paper, we proposed tungsten complex gratings with different three groove depths as near-infrared TPV wavelength selective emitters under TM wave incidence. The influence of different filling ratios, incident angles and groove depths on the spectral emittance of tungsten grating was firstly studied by using numerical calculations rigorous coupled wave analysis. Then the performance of the complex gratings was compared with simple gratings.

2. Design of the Complex Grating

Figure 1 (a) shows a TM wave with wavevector k, incident from air on a 1D simple binary grating. The material of the grating ridges and the substrate is tungsten (W). The wavevector can be decomposed into two components, k_x and k_z, along the x- and z-axis, respectively. The magnetic field H oscillates perpendicular to the plane of incidence and parallel to the grating grooves. The magnetic field H oscillates perpendicular to the plane of incidence and parallel to the grating grooves. The geometric parameters of the simple grating can be depicted by its period Λ , groove depth (ridge height) h , ridge width d and groove width t as shown in Figure 1 (a). The grating period (Λ) is composed of only one ridge and one groove, *i.e.*, $\Lambda = d + t$ and $d = f\Lambda$, $t = (1 - f)\Lambda$, where f is the filling ratio. Figure 1 (b) shows concave complex gratings with different three groove depths. It contains three simple gratings in a period with ridge widths d_1, d_2 and d_3 , groove widths t_1, t_2 and t_3 , and groove depths h_1, h_2 and h_3 . The angle θ is the corresponding emission angle. The emittance is calculated indirectly from the reflectance, based on Kirchhoff's law. The wavelength range of radiation from 0.3 μm to 4 μm is of interest to the selected system in this study.



Simple Grating



Complex Grating

Figure 1. Schematic Diagram of a Binary 1D Tungsten Simple Grating and Concave Complex Tungsten Grating for a TM Wave Incident from Air at an Incident Angle θ ona Simple Grating (b) Complex Grating with Three Different Groove Depths

3. Calculation Method

Rigorous coupled-wave analysis (RCWA) is formulated in the 1980s by Moharam and Gaylord. It is used for analyzing the diffraction of electromagnetic waves by periodic gratings [24]. RCWA is used in this study to calculate the radiative properties (emittance and transmittance) of the periodically multilayer surfaces. It analyzes the general 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. For simplicity, the plane of incidence is set to be perpendicular to the grating grooves in the present study. The optical properties of tungsten at room-temperature, used in the RCWA calculation, are taken from Ref. [26].

4. Simulation Results and Discussion

4.1. Effect of Filling Ratio on Emittance

The normal emittance of 1D simple binary tungsten gratings with grating period of $\Lambda = 0.8\mu m$, depth of the groove of $h = 0.1\mu m$, at incident angle $\theta = 0^\circ$ and different filling ratios for TM waves is shown in Figure 2. It can be seen that the normal emittance of tungsten gratings with different filling ratios are much larger than that of plain tungsten (*f* = 0 or 1) due to surface Plasmon polaritons excitation SPPs. It has to be noted that the wavelength and magnitude of the peak strongly depend on the filling ratio f . When the filling ratio increases, the peak shifts toward longer wavelength while at $f = 1$, the emittance decreases, which also corresponds to the plain tungsten.

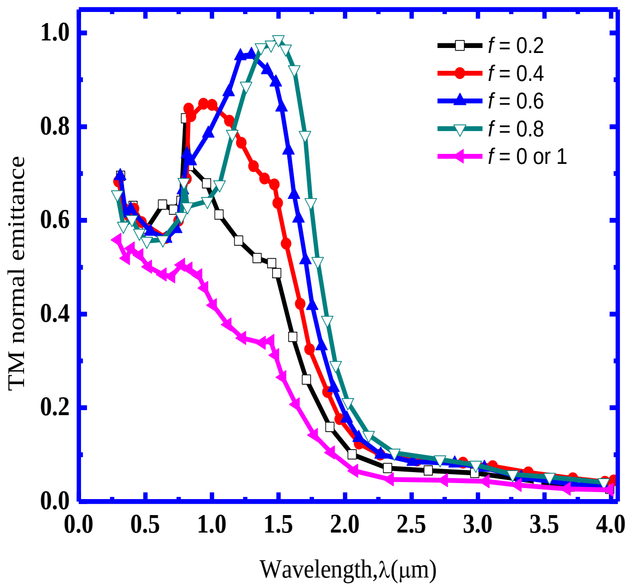


Figure 2. Simulated Normal Emittance of Simple Gratings with Different Filling Ratios for TM Waves

4.2. Effect of Incident Angle on Emittance

Figure 3 illustrates simulation results for the spectral emittance of simple tungsten grating for TM waves with different incident angles. The geometrical parameters of the gratings are depicted as period of grating $\Lambda = 0.8\mu m$, $f = 0.5$, $d = t = 0.4\mu m$ and $h = 0.2\mu m$. It can be noted that as the incident angle increases, the emittance decreases and the peak shifts toward longer wavelength, and becomes very sharp. The results show that all curves have peaks at $\lambda = 0.36\mu m$, $\lambda = 0.73\mu m$, and the curves with $\theta = 60^{\circ}$ and $\theta = 75^{\circ}$, have another obvious peak at $\lambda = 1.5\mu m$. The curves almost coincide when $\theta = 60^{\circ}$ and $\theta = 75^{\circ}$. The results show the spectral emittance peak of simple tungsten grating depends on the incident angle.

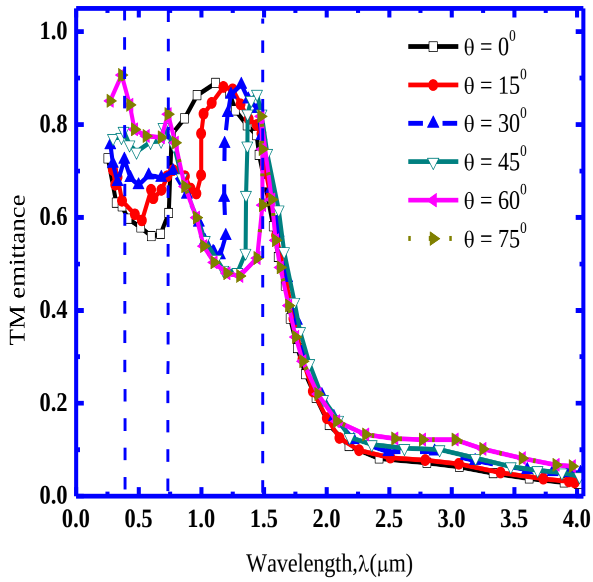


Figure 3. Simulated Spectral Emittance of Simple Gratings with Different Incidence Angles for TM Waves

4.3. Effect of Groove Depths on Emittance

The normal emittance of the simple tungsten gratings, when $\Lambda = 0.8\mu m$, $f = 0.4$ and different groove depths $h = 0\mu m$, $0.05\mu m$, $0.1\mu m$ and $0.2\ \mu m$ at $\theta = 0^{\circ}$ for TM wave are shown in Figure 4.The results show that the emission peaks are broadened and shifted towards longer wavelengths when the groove depth is increased. Note that the emittance does not always increase with the groove depth, and the largest groove depth does not correspond to the largest emittance. This indicates that there is an optimal groove depth in a specified geometry grating, and peak wavelength and value are highly sensitive to groove depth. A high emittance from the visible and near- infrared region like this is suited to TPV emitters. So we propose new concave complex gratings, as shown in Figure 1(b), with different groove depths to improve emittance and makes it broader in the visible and near-infrared regions.

5. Complex Grating Performance

The thermophotovoltaic emitters usually work at an elevated temperature and their emissivity should be high, close to unity, at wavelengths between 0.8 and 1.7 μm , where a TPV cell (GaSb) has high quantum efficiency. Figure 5 shows the comparison of spectral emittance between simple tungsten gratings with different groove depths and the complex grating at emission angle $\theta = 0^{\circ}$ for TM and TE waves, respectively. The widths of ridges and grooves are the same ($d_1 = d_2 = d_3 = d$ and $t_1 = t_2 = t_3 = t$) for the complex gratings, and $d = t = 0.4\mu m$ for all simple gratings and complex gratings. The groove depths of the simple tungsten gratings are $h = 0\mu m$, 0.05 μm , 0.1 μm and 0.2 μm .From Figure 5 (a), it can be seen that complex gratings with different groove depths can enhance the emittance for TM wave by the excitation of surface plasmon polaritons compared to the simple grating. The emittance of complex gratings is above 0.9 at $\lambda = 1.76\mu m$ .The simulation results show that the complex gratings is suitable to a TPV selective emitter with a low bandgap photovoltaic cell (GaSb) to improve TPV efficiency and enhancement electrical output power. The results in Figure 5 (b) exhibits just a little enhancement in the emittance for complex gratings compared with simple gratings for TE-polarized wave, which is also unobvious as that for TM-polarized wave.

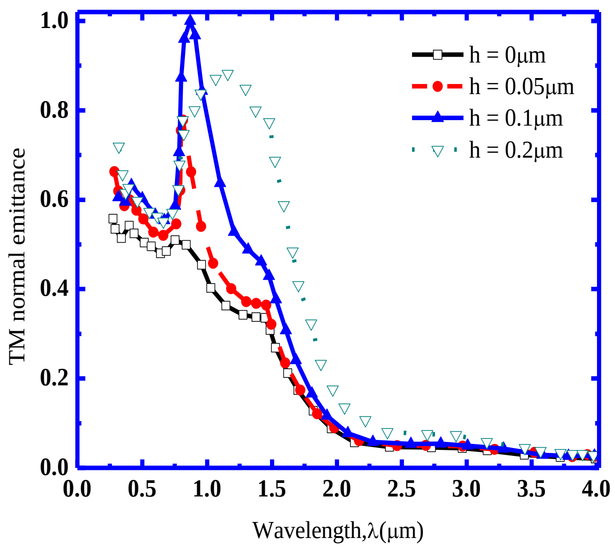


Figure 4. Simulated Normal Emittance of Simple Gratings with Different Groove Depths for TM Waves

Figure 6 (a) and (b), displays the comparison of spectral emittance between plain tungsten, simple tungsten gratings and the complex gratings at emission angle $\theta = 0^{\circ}$ and 60° for TM waves. The normal emittance of plain tungsten is not high enough at short wavelengths such that it cannot be a good TPV emitter. The results show that the emittance of the gratings has peaks at the spectral region of 0.8 $\mu m \le \lambda \le 1.76\mu m$. The emittance of simple grating is high in a broad spectral region. The emittance peak of the complex grating at normal emission is wider than that of simple grating, especially at long wavelengths. The peak value of the complex grating is higher than 0.9 at $\lambda = 1.76\mu m$ and lower than 0.2 at $\lambda \ge 2.2\mu m$. It is also a little higher than that of the plain tungsten at short wavelengths due to the surface microstructures effect to reduce reflectance and enhance emission for TM waves. However, the emittance is still much lower than the peak and the performance as TPV emitters but, the normal emittance of the complex grating gives promising results.

The emittance at short wavelengths ($\lambda \leq 1\mu m$) at $\theta = 60^{\circ}$ is higher than that at $\theta = 0^{\circ}$ for plain tungsten and tungsten gratings as shown in Figure.6 (b).The results show there are no difference in the emittance of plain tungsten and tungsten simple gratings at $\theta = 60^{\circ}$ except only significant difference is the peak at $\lambda \approx 1.5\mu m$ for simple grating due to the SPP excitation. The complex grating at $\lambda \approx 1.5\mu m$, it is also has emittance peak. Furthermore, the emittance of the complex grating is the highest at $\lambda > 0.75\mu m$ with values exceeding 0.7 at $\lambda < 1.73\mu m$ and lower than 0.2 at $\lambda \geq 2.2\mu m$. Hence, the complex grating is suitable to use as a TPV selective emitter at large emission angles.

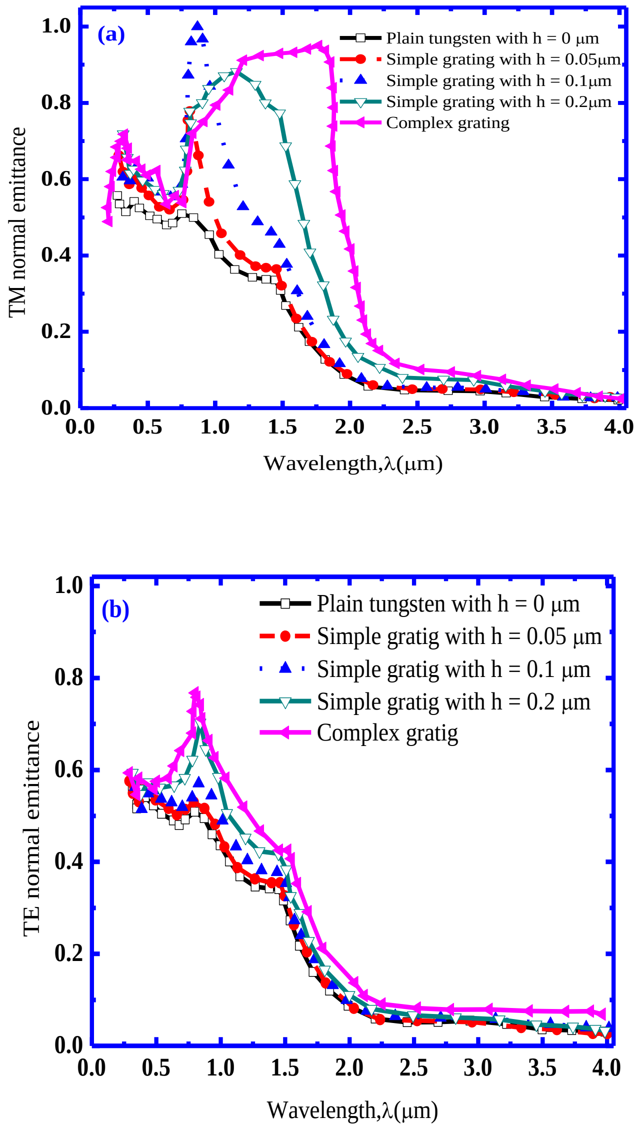
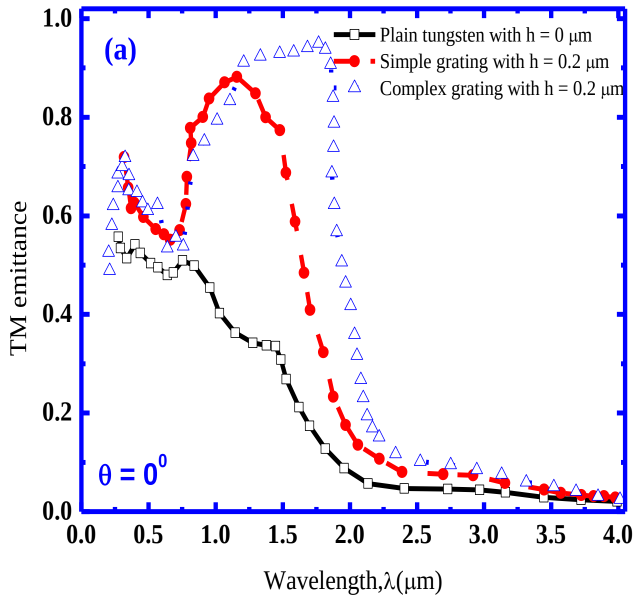


Figure 5. Simulated Normal Emittance of Complex Gratings Compared with that of Simple Gratings for (a) TM Waves (b) TE Waves



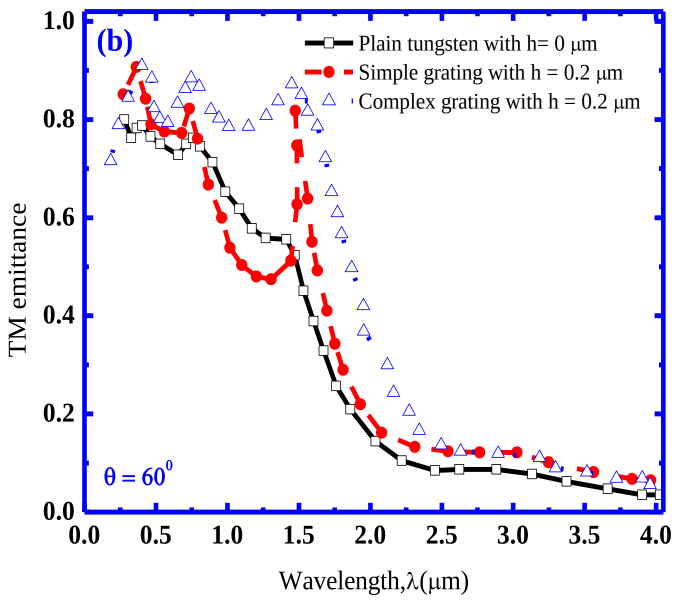


Figure 6. Simulated Spectral Emittance of Plain Tungsten and Tungsten Gratings for TM waves at (a) $\theta = 0^{\circ}$ **(b)** $\theta = 60^{\circ}$

6. Conclusion

The effect of the geometric parameters such as filling ratio, incident angle and groove depth on the spectral emittance of the simple tungsten grating is investigated by rigorous coupled-wave analysis (RCWA) method. There are optimal filling ratio and groove depths in a specified geometry grating. The spectral emittance peak of simple tungsten grating depends on the incident angle. A 1D tungsten complex grating is proposed for potential application as thermophotovoltaic selective emitter working at wavelengths between 0.8 and 1.7 μm . It has three groove heights in one period. The emittance enhancement for TM waves can be explained by the excitation of surface plasmon polaritons coupled with the grating microstructures. The emittance of the complex grating numerically exhibits a wide peak in our wavelength of interest but lower than 0.2 at $\lambda \geq 2.2 \mu m$. The performance of the complex grating with different polarization and incident angle is also studied for comparison between plain tungsten and simple tungsten gratings. The complex grating can be used as a selective emitter for TPV applications.

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Authors

Samah G Babiker, is a PhD student in Harbin Institute of Technology, School of Energy Science and Engineering, Harbin-China. She received an MSc degree in solid state physics from Sudan University of Science and Technology -Khartoum -Sudan in 2009, an BSc degree in Physics Laboratory from the same university in 2006. Her research area of interest is thermo physics, nano/microscale heat transfer.

Mohamed Osman Sid – Ahmed, received Ph. D degree in Solar Energy from University of Reading (U.K) in 1981, an MSc degree in Meteorology in 1970, B. Sc degree in Physics in1967 from the same university Reading- U.K. He worked in department of Meteorology-Khartoum-Sudan from1970-1975. From1975-1986 he was Researcher in the Energy Research Institute and National Council for research Khartoum-Sudan. From 1986 -1990, he was an associate Professor and Head of the Applied Physics department- University Gezira-Sudan. From 1990-1994, he was an associate Professor and Head of Wind Energy Department, National Centre for Research, Khartoum-Sudan. From 1994-1996, he was, Dean of Faculty of Education, University of El-Fashir-Sudan. From 1997-2003 he was, Head of physics Department., Hail T. College, Saudi Arabia.From2003-2005 he was, Head of physics Department- Sudan Univ. of Science and Technology .He is currently a professor of physics, Physics Dept., Sudan Univ. of Science and Technology, Khartoum-Sudan. His research interests are radiative heat transfer and organic solar cells, Renewable Energy.

Yong Shuai, is an associate professor at Harbin Institute of Technology. He got his PhD degree from Harbin Institute of Technology in 2009. He worked as a visiting scholar in 2011-2012 at Georgia Institute of Technology. His research is centered on nano/microscale heat transfer, and solar thermal utilization.

Ming Xie, received the Ph.D. degree in School of Energy Science and Technology from Harbin Institute of Technology (HIT) in Harbin, China in 2006. From 1984 to 1986, he worked at HIT as an associate engineer. From 1986 to 1994, he was a lecturer at the Department of Civil Engineering of HIT. From 1995 to 2001, he was an associate professor at the Department of Civil Engineering, HIT, and served as the vice president of this department during 1997 to 2000. He is currently a professor of engineering thermal physics at School of Energy Science and Technology, Harbin Institute of Technology, China. His research interests are radiative heat transfer and coupled heat transfer, surface radiation and particle radiation characteristics, target infrared model, and air conditioning systems.