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Optimal Design of Wavelength Selective Thermal Emitter for Thermophotovoltaic Applications

We theoretically and numerically demonstrate optimal design of wavelength selective thermal emitter using one-dimensional (1D) and two-dimensional (2D) metal-dielectric gratings for thermophotovoltaic (TPV) applications. Proposed design consists of tungsten (W) and silicon dioxide (SiO₂) gratings which can withstand high temperatures. Radiative properties of 1D grating were calculated using a numerical method, while effective medium approximation was used for 2D gratings. Optimal designs were obtained such that output power is maximum for GaSb photovoltaic (PV) cell at emitter temperature of 1500 K and radiated energy for longer wavelengths is limited to a low value. A constrained optimization was performed using genetic algorithm (GA) to arrive at optimal design. [DOI: 10.1115/1.4036790]

1 Introduction

Thermophotovoltaics (TPV) technology has promising applications in waste heat recovery [1] as well as in solar power generation [2]. TPV offer clean and quiet electricity generation and, therefore, could be competing alternative to existing electricity generation plants [3]. A TPV system consists of an emitter which receives thermal energy from a heat source and emits radiation, and a photovoltaic cell that generates electricity from incident photons [4]. While ideal TPV systems with monochromatic radiation can achieve Carnot efficiency [5–8], in reality, TPV performance is significantly limited by the mismatch that arises between emission spectrum of emitter and absorption spectrum of the photovoltaic (PV) cell [9]. PV cell characteristics are defined by external quantum efficiency (EQE) that denotes the fraction of incident photons converted into electron-hole pairs [10] and is directly proportional to amount of current produced for a given incident wavelength. A PV cell can generate electric current only when energy of incident photon is higher than bandgap of the material [11], i.e., when EQE has a nonzero value. Absorption of incident photons having energy lower than bandgap (wavelength higher than bandgap wavelength) leads to thermal leakage causing inefficiency and, therefore, is undesirable. So, an optimal thermal emitter would have maximum thermal emission in the region of high EQE and limited emission for lower energies. Goal is to develop a wavelength selective emitter that targets particular range of wavelengths to match with a PV cell. Plasmonic metamaterials [12], photonics crystals [13,14], single micro/nano sized spheres [15], nanoparticle-embedded thin-films [16], doped materials [17,18], and surface gratings are possible candidates to obtain spectrally selective emission [19]. Metamaterials [20] and 1D, 2D, and 3D photonic crystals are focus of several studies dealing with TPV systems [21–23].

In present work, we propose grating-based design of selective thermal emitter specifically aimed for GaSb type of PV cell.

Figure 1 displays two distinct types of designs considered here. One with 1D gratings (Fig. 1(a)) and another with 2D gratings (Fig. 1(b)). Both designs consist of a thin grating layer of W and SiO₂ on W substrate. For 1D grating, grating period Λ , filling ratio ϕ , and grating thickness t can be varied to change spectral response of the structure. For the symmetric 2D grating considered, filling ratio ϕ and grating thickness t are the parameters of interest while grating period Λ is fixed to be 100 nm. The objective of this work is to put forward an optimization method to arrive at best design for given constraints and operating temperature. This is achieved by MATLAB-based genetic algorithm tool. Goal of optimization is to maximize output power by the PV cell and to limit the losses.

2 Theoretical Fundamentals

The hemispherical emissivity of an opaque material is given by [16]

$$e(\omega) = \frac{c^2}{\omega^2} \int_0^{\omega/c} dk_p k_p \sum_{\mu=s,p} \left(1 - |\tilde{R}^{(\mu)}|^2\right) \quad (1)$$

where c is the speed of light in vacuum, ω is the angular frequency, and k_p is the magnitude of inplane wave vector. $\tilde{R}^{(\mu)}$ is the polarization-dependent effective reflection coefficient, and hence, $|\tilde{R}^{(\mu)}|^2$ is the reflectivity of the surface. Here, $\mu = s$ (or p) refers to transverse electric (or magnetic) polarization. The dielectric functions can be related to complex refractive index as $\sqrt{\epsilon} = n$. Dielectric functions of the materials (SiO₂ and W) considered in this paper are taken from literature [24,25]. Having very low temperature coefficients, room temperature values of dielectric function are used for SiO₂ [26]. Dielectric properties of tungsten were also assumed to be independent of temperature as the operating temperature is much less than its melting point.

For diffraction gratings, reflectivity $|\tilde{R}^{(\mu)}|^2$ is summation of reflectance of all diffraction orders [27]. In order to calculate reflectivity of 1D grating structure, we employ numerical method to obtain solutions to Maxwell's equations using rigorous coupled

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Fig. 1 Schematics of proposed designs consisting W/SiO₂ gratings on W substrate: (a) a 1D rectangular grating and (b) symmetric 2D grating

wave analysis (RCWA). A MATLAB-based code developed by Nanoscale Thermal Radiation Laboratory at Georgia Institute of Technology was used for this purpose. Fifty diffraction orders were found to be sufficient for calculation of reflectivity for range of 1D designs considered in the study.

For symmetric 2D gratings, we use effective medium approximation to calculate effective refractive index of the top layer. For symmetric 2D grating consisting two media having dielectric functions ϵ_1 and ϵ_2 (refractive indices n_1 and n_2 , respectively) and filling ratio f of medium 2 in medium 1, effective refractive index of the medium is given by [28]

$$n_{2D} = [\bar{n} + 2\hat{n}_{2D} + 2\check{n}_{2D}]/5 \quad (2)$$

where $\bar{n}$, $\hat{n}_{2D}$, and $\check{n}_{2D}$ can be obtained using

$$\bar{n} = (1 - f^2)n_1 + f^2n_2 \quad (3)$$

and

$$\hat{\epsilon}_{2D} = (1 - f)\epsilon_1 + f\epsilon_{\perp} \quad (4a)$$

$$1/\check{\epsilon}_{2D} = (1 - f)/\epsilon_1 + f/\epsilon_{\parallel} \quad (4b)$$

where $\epsilon_{\perp}$ and $\epsilon_{\parallel}$ are given by

$$\epsilon_{\parallel} = (1 - f)\epsilon_1 + f\epsilon_2 \quad (5a)$$

$$1/\epsilon_{\perp} = (1 - f)/\epsilon_1 + f/\epsilon_2 \quad (5b)$$

Reflectance coefficient of the structure is calculated using Fresnel equations [29] that can be used to calculate emissivity. As effective medium approximation is valid for grating periods much smaller than the wavelength of interest, we limit ourselves to $\Lambda = 100$ nm for 2D gratings and keep this parameter fixed during optimization.

3 Optimization

Emissivity of a typical thermal emitter is shown by the black curve in Fig. 2. Dashed line denotes EQE of GaSb cell. Although comparison of emission spectrum of the emitter and the EQE curve of the PV cell can be a good indicator of TPV system's performance, the emitter temperature has a critical role as it decides the dominant thermal wavelength and can dictate the overall efficiency. Radiated heat flux by the thermal emitter is given by

$$P_{\text{rad}} = \int_0^{\infty} \frac{\omega^2}{4\pi^2 c^2} \frac{\hbar\omega}{(e^{\hbar\omega/k_B T} - 1)} e(\omega) d\omega \quad (6)$$

where $\hbar$ is Planck's constant, k_B is Boltzmann's constant, T is the emitter temperature, and $e(\omega)$ is the emissivity of the emitter. Emitted power at 1500 K is shown by the solid curve below dashed one in Fig. 2. The power output, P_{out} , is proportional to the number density of the photons above bandgap and the EQE of PV cell defined as [30]

$$P_{\text{out}} = qV_{\text{OC}}\text{FF} \int_0^{\infty} \bar{n}(\omega, T) e(\omega) \eta_{\text{EQE}}(\omega) d\omega \quad (7)$$

where q , V_{OC} , FF, and η_{EQE} are electronic charge, open circuit voltage, fill factor, and EQE of PV cell, respectively. $\bar{n}(\omega, T)$ is the number density of incident photons given by

$$\bar{n}(\omega, T) = \frac{\omega^2}{4\pi^2 c^2} \frac{1}{(e^{\hbar\omega/k_B T} - 1)} \quad (8)$$

Shaded green region in plot shows the output power of PV cell, while dashed cyan line shows maximum available power that can be extracted by an ideal PV cell. Note that realistic values of V_{OC} and FF are used to obtain P_{out} in Fig. 2. As PV cell generates current only for nonzero values of EQE, energy radiated below the band gap is wasted (denoted by shaded red area). One can design

Fig. 2 Emission spectrum of a typical thermal emitter is shown in comparison with EQE of GaSb cell. Spectral heat flux, maximum available heat flux, and power output are calculated at emitter temperature of 1500 K and typical values of V_{OC} and FF.

an optimal emitter by maximizing the ratio of P_{out} to P_{rad} , and therefore maximizing the overall efficiency. Alternatively one may optimize effectiveness index [20]. However, losses due to long wavelength photons not only contribute to inefficiency but they also lead to heating of PV cell which can be potentially bad for malfunction of PV cell. Therefore, we choose a constrained optimization approach, wherein we maximize output power and limit the waste heat. Losses are limited to that of an emitter with emissivity 0.1. If ω^* is the angular frequency corresponding to the bandgap of PV cell, optimization can be formulated as follows:

$$\text{maximize } \int_0^\infty \bar{n}(\omega, T) e(\omega) \eta_{\text{EQE}}(\omega) d\omega \quad (9)$$

subject to: nonlinear constraint

$$\int_{\omega^*}^\infty \frac{\hbar\omega^3}{4\pi^2 c^2} \frac{e(\omega) d\omega}{(e^{\hbar\omega/k_B T} - 1)} \leq \int_{\omega^*}^\infty \frac{\hbar\omega^3}{4\pi^2 c^2} \frac{0.1 d\omega}{(e^{\hbar\omega/k_B T} - 1)} \quad (10)$$

Genetic algorithm (GA) was used to maximize the objective function subject to the constraints. A MATLAB-based optimization tool was utilized to perform optimization. The algorithm to determine optimal emission spectrum can be described as follows:

- (1) For emitter temperature of $T=1500$ K range of wavelengths, EQE and number of wavelengths for calculation of emission spectrum and objective function are fixed.
- (2) Genetic algorithm:
 - (i) Initial random population of independent variables (ϕ, Λ, t for 1D and ϕ, t for 2D gratings) is generated.
 - (ii) For each set of independent variable, objective function is calculated using Eq. (9). RCWA method is used for 1D grating, while effective medium approximation is used for 2D grating. Each set is ranked based on the value of objective function.
 - (iii) Some sets independent variables from population are selected to be parents based on their ranks.
 - (iv) Offsprings of independent variables are generated by crossover of parents' variables.
 - (v) Mutations are performed on offsprings variables.
 - (vi) Variables from parent population are randomly replaced by offspring population.
 - (vii) Steps (ii)–(vi) are repeated until the average change in the value of objective function over stall generations is less than user-specified tolerance.

4 Discussion and Results

The following MATLAB-prescribed options are selected in the genetic algorithm toolbox for the purpose of optimization in this paper:

- Population type: double vector with populations size = 50.
- Fitness scaling: rank.
- Selection function: stochastic uniform reproduction.
- Reproduction: elite count: 0.05, crossover fraction: 0.8.
- Mutation function: Constraint dependent.
- Crossover function: Constraint dependent.
- Migration: direction: forward, fraction: 0.2, interval: 20
- Algorithm settings: as default.
- Stopping criteria: generations: 100.

There are additional linear constraints for optimization of 1D grating-based design

$$0.1 \leq \phi \leq 0.9 \quad (11a)$$

$$50 \text{ nm} \leq \Lambda \leq 2 \mu\text{m} \quad (11b)$$

$$50 \text{ nm} \leq t \leq 2 \mu\text{m} \quad (11c)$$

Fig. 3 Spectral response of 1D and 2D optimal designs in comparison with EQE of GaSb cell. Emission spectra of suboptimal designs are shown for reference. (1D suboptimal: $\Lambda = 0.5 \mu\text{m}$, $\phi = 0.3$, and $t = 0.5 \mu\text{m}$; 1D optimal: $\Lambda = 446 \text{ nm}$, $\phi = 0.17$, and $t = 630 \text{ nm}$; 2D suboptimal: $\Lambda = 100 \text{ nm}$, $\phi = 0.1$, and $t = 0.5 \mu\text{m}$; 2D optimal: $\phi = 0.71$ and $t = 95 \text{ nm}$.)

$$0.5\Lambda \leq t \leq 2\Lambda \quad (11d)$$

Equations (11a)–(11c) set realistic bounds, while Eq. (11d) makes sure that the geometry of grating layer is not disproportionate. Parameters for 2D grating are ϕ and t . So, linear constraints are

$$0.1 \leq \phi \leq 0.9 \quad (12a)$$

$$50 \text{ nm} \leq t \leq 2 \mu\text{m} \quad (12b)$$

The thermal emitter designs considered in the study are suitable for TPV system consisting of GaSb-based photovoltaics. The EQE of GaSb cell is shown in Fig. 3. GaSb cell efficiently generates electricity if the wavelength of incident photons falls between $0.4 \mu\text{m}$ and $1.88 \mu\text{m}$. Figure 3 shows emission spectra of the two optimal designs of thermal emitter obtained using optimization method discussed earlier. Optimal design (shown by black dashed line) of 1D grating has a grating period of 446 nm , filling ratio of 0.17 , and grating thickness of 630 nm . Two-dimensional optimal design (line with asterisk) has a grating period of 100 nm , filling ratio of 0.71 , and grating thickness of 95 nm . Both 1D design as well 2D design exhibit high emissivity (>0.8) in the wavelength range 0.4 – $1.88 \mu\text{m}$ and very low emissivity (<0.2) beyond $2 \mu\text{m}$. The radiated power beyond $1.88 \mu\text{m}$ is less than that of an emitter having emissivity of 0.1 . A high conversion efficiency is ensured due to close match between the emission spectra of the emitter and EQE of the PV cell minimizing thermal leakage of long wavelength photons. Although substantial part of blackbody radiation at temperature of 1500 K exists beyond $1.88 \mu\text{m}$, very little heat is wasted in this region as emissivity is low. This indicates lower losses due to thermal leakage. For comparison, suboptimal designs of 1D (green dash-dot line) and 2D (blue line with circle) grating structures are shown. One-dimensional suboptimal design has a grating period of $0.5 \mu\text{m}$, filling ratio of 0.3 , and grating thickness of $0.5 \mu\text{m}$, while 2D suboptimal design has a grating period of 100 nm , filling ratio of 0.1 , and grating thickness of $0.5 \mu\text{m}$. For quantitative comparison of optimal and suboptimal designs, Table 1 shows radiated power, output power, overall efficiency, and effectiveness index calculated at emitter temperature of 1500 K . Effectiveness index is calculated using the definition [20]

Table 1 Comparison of emitter performance for optimal and suboptimal designs of 1D and 2D gratings corresponding to Fig. 3

		P_{rad} (W/m ²)	P_{out} (W/m ²)	$\frac{P_{\text{out}}}{P_{\text{rad}}}$	β_{emitter}
1D	Suboptimal	45,131.7	8258.9	0.18	0.96
	Optimal	50,130.7	9492.3	0.19	0.99
2D	Suboptimal	43,595.1	6370.1	0.15	0.76
	Optimal	67,744.2	10,497.1	0.15	0.81

$$\beta_{\text{emitter}} = \left(\frac{P_{\text{out}}}{P_{\text{rad}}} \right)_{\text{Real}} \times \left(\frac{P_{\text{rad}}}{P_{\text{out}}} \right)_{\text{Ideal}} \quad (13)$$

Notice that in both cases, optimal and suboptimal designs have similar values of overall efficiency. However, optimal designs have higher output power and are closer to an idealized emitter. Poorer performance of both suboptimal designs can be also observed from the mismatch between their emission spectra and corresponding EQE in Fig. 3.

5 Conclusions

Thus, we have presented two designs of thermal emitters, namely, 1D grating-based and 2D symmetric grating-based emitters for GaSb based PV cell. RCWA-based numerical method was used to calculate emission spectra of 1D designs, while effective medium approximation was employed to calculate spectral response of 2D structures. Spectral tuning of emission was achieved by varying parameters such as grating period, filling ratio, and grating thickness. An optimization method is proposed that utilizes GA to maximize output power of the TPV system while limiting the losses due to thermal leakage. Emission spectra of optimal designs obtained using this method for emitter temperature of 1500 K matches well with the EQE of PV cell. Materials chosen for design are suitable for high operating temperatures. This study gives valuable insights into design and optimization methods for selective thermal emitters for TPV systems.

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