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Four-layer metallodielectric emitter for spectrally selective near-field radiative transfer in nano-gap thermophotovoltaics

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ABSTRACT

A four-layer metallodielectric planar thermal emitter is designed and optimized to tailor the spectral near-field radiative flux in a nano-gap thermophotovoltaic (TPV) system. The structure contains an ultra-thin refractory metallic layer (tungsten) sandwiched by two dielectric (hafnia) layers sitting on a metallic substrate. The theoretical calculation showed that the lossy metallic thin-layer acted as a perfect absorber that stimulated strong thermal emission, with its frequency and amplitude further modulated by the Fabry–Perot resonances in the dielectric layer. The spectral peak of near-field radiative flux can be manipulated by layer thickness to suit different cell bandgaps and emitter temperatures. The combination of optimized emitter and cell layer thickness results in selectively high near-field radiative flux above the bandgap, reaching a conversion efficiency of 50.2% (at radiative limit) with emitter temperature at 1600 K and 200 nm vacuum gap, surpassing or comparing with the efficiency and output power of state-of-the-art plasmonic and hyperbolic emitter designs. By tailoring the radiative heat flux mainly in the propagating and frustrated components, the design also circumvents possible electrical losses due to enhanced surface recombination when the radiative transfer is dominated by surface modes. This study offers a straightforward strategy to manipulate the near-field radiative transfer with great flexibility by a few-layer planar emitter and emphasizes the different consideration for designing a nano-gap TPV emitter from far-field PV/TPV emitter designs.

1. Introduction

Thermophotovoltaic (TPV) systems are energy conversion devices that transform thermal radiative emission from a high-temperature emitter to electricity by using the photovoltaic effect of semiconductors [1]. The key components of TPV are semiconductor cell and thermal emitter, separated by a vacuum gap to ensure that heat is transferred between them only through thermal radiation. The emitter is heated by external heat sources, such as solar power [2,3], industrial waste heat [4], and decay of radioisotopes [5], resulting in the thermal emission of photons. Photons absorbed by TPV cell with higher energy than the bandgap generate electron/hole pairs (EHPs), which are converted to output electricity. With its capability to use versatile heat sources and potentially high conversion efficiency, TPV is a promising candidate for next-generation power generation systems. A nano-gap TPV system [6,7] shrinks the gap between the emitter and cell to a sub-micrometer scale to utilize the evanescent components of thermal radiated electromagnetic (EM) waves, that is, the near-field radiative heat transfer phenomenon [8]. The extreme proximity of the emitter and absorber increases the possibility of photons tunneling through the gap, which enables the total radiative flux to surpass the upper limit for far-field radiative transfer governed by the Planck equation at given temperature. Experimental investigations notably from DiMatteo et al. [9] and Hanamura et al. [10,11] indicated that narrowing the vaccum gap to sub-micrometer scale enhanced the short-circuit current of the TPV device, while theoretical analysis on the physics for energy manifesting and losses in a nano-gap TPV can be found in Refs [12–30].

The power and efficiency performance of TPV highly depend on the spectral radiative properties of the thermal emitter and cell. The aim is to design a spectrally matched pair of thermal emitter and absorber (TPV cell), which makes the radiative transfer through the vacuum gap selectively high at a frequency slightly above the cell bandgap [31]. Although a wide range of emitter designs have been investigated for far-field TPV, limited designs aimed specifically at tailoring the near-field radiative transfer in

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nano-gap TPV. This condition is partly attributed to the extremely narrow gap in near-field radiative transfer that hinders several applicable approaches for shaping thermal emission, such as by using selective filters [32,33]. However, the presence of evanescent waves opens the possibility for new mechanisms on spectral manipulation, such as by surface plasmon polaritons (SPP) [34], magnetic polaritons [35], and hyperbolic metamaterials (HMM) [36,37]. Many of the proposed thermal emitters are realized by complex nanostructures, which may be difficult for large-scale fabrication and may have limited thermal stability under a high working temperature. Comparatively, a simple planar selective emitter design has the significant potential to decrease the cost and boost the endurance of a practical nano-gap TPV system. Representative designs on planar emitters for nano-gap TPV include bulk [24] and single layer thin-film [25] planar plasmonic emitter, single layer ultrathin semiconductor as a "thermal-well" [22], infinite periodic layers HMM [29,38], and the application of 2D materials such as graphene [39,40].

An interesting strategy for designing a thermally stable planar emitter for TPV application is a few-layer planar structure, which has the potential to offer greater design flexibility than bulk or single layer thin-film designs, while still keeping the practical fabrication simple enough. Specifically, a few-layer metallodielectric structure with alternating metallic and dielectric layers can be used for shaping the spectral radiative transfer. The lossy metallic layer can be tailored for narrowband or broadband high emissivity via the coherent perfect absorption [41]. The dielectric layers act as Fabry–Perot (F–P) resonant cavities for manipulating the spectral and angular emissivity of the structure. The design principle has been theoretically analyzed for far-field applications [42], and the structural stability is experimentally proven over 1500 K by selecting components with high melting points and matching thermal expansion coefficients [43,44]. In a recently publication, Blandre et al. [45] discussed a Mo–HfO_2 four-layer structure as a far-field TPV emitter and presented detailed analysis on how the designed layer thickness manipulated the phase of radiative flux and thus manipulating the spectral thermal emissivity. For a nano-gap TPV system operating at near-field distances, however, a few-layer metallodielectric emitter has not been discussed as most designs only accounted for normal emissivity/absorptivity and a few cases considered the wide-angle robustness of emissivity [46–51], yet the near-field radiative transfer is largely dependent on evanescent modes with large lateral wavevector that is inexistent for far-field radiative transfer cases. Moreover, the thermal radiative contribution from individual layers might differ in the near-field scenario because the gap size between the emitter and absorber becomes comparable with the emitter layer thickness. Considering these reasons, structures that enhance the far-field radiative transfer might not work for near-field cases [52] and vice versa.

Therefore, this study designed a four-layer metallodielectric emitter specifically for nano-gap TPV applications. The spectral radiative transfer from the emitter to a thin-film InGaAsSb cell absorber is effectively manipulated by using an ultrathin tungsten layer sandwiched by two dielectric layers sitting on a metallic substrate. This study revealed the physical mechanism for metallodielectric emitter to stimulate high spectral radiative flux in a narrow spectral range above the bandgap of the cell by investigating the pattern of energy transfer coefficient along frequency and lateral wavevector, in which special attention is paid to the difference from designing a far-field selective emitter. A detailed walkthrough showed the tailoring of the thickness of individual layers to match the bandgap of the cell for optimizing TPV efficiency as calculated in the radiative limit, surpassing the system performance of other state-of-the-art emitter proposals. The structural design and optimization approach aided in designing a multilayer metallodielectric emitter for achieving high conversion efficiency and output power of nano-gap TPV system.

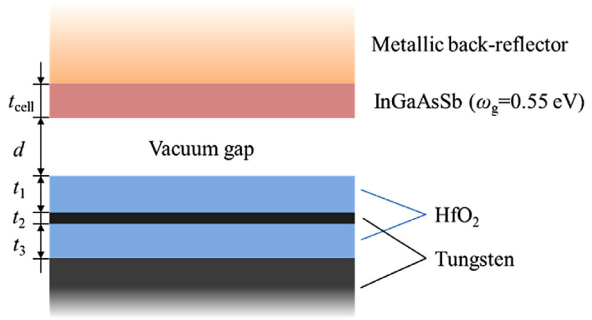

Fig. 1. Proposed system structure.

2. Theoretical model

2.1. Geometry and material

The studied system is shown in Fig. 1. The four-layer metallodielectric emitter consists of an ultrathin metallic layer sandwiched by two dielectric layers sitting on a metallic substrate. Tungsten (W) and hafnia (HfO_2) are selected as the component materials following the same principle for the design of a far–field selective emitter. The bulk and thin-film of W are frequently modeled as TPV emitters [20,53] due to the high melting point and high loss. HfO_2 is a transparent dielectric material tested as a high–temperature protection layer for refractory metals with satisfactory thermal stability [54,55]. The sandwiched tungsten layer provides the high emitting/absorbing power required for a TPV emitter, and the two dielectric layers act as F–P cavities to maneuver the frequency and amplitude of the peak radiative flux, presented in detail in Section 3.

The absorber is an ultrathin layer InGaAsSb cell with a bandgap of $E_g = \hbar\omega_g = 0.55$ eV as measured at room temperature [56], sitting on a metallic back-reflector. The combination of an ultrathin cell with a reflective metallic substrate is designed to suppress the absorber reflection by tailoring the phase shift inside the semiconductor layer. In practice, the fabrication of ultrathin layers of III–V alloy have been demonstrated [57] and direct fabrication on a metallic substrate is also possible [58].

For the material permittivity used in the calculation, the permittivity of W is determined by a temperature-dependent Drude–Lorentz model [59]. For HfO_2, $\varepsilon_{HfO_2} = 4 + 0i$ is assumed in the studied spectral region according to the measured data by Bright et al. [60]. The permittivity of the InGaAsSb is characterized by the model of Gonzalez–Cuevas et al [61] for III–V quaternary alloys. The metallic back-reflector takes the properties of gold (Au) at room temperature measured by Johnson and Christy [62].

2.2. Calculation of near-field radiative transfer

The radiative transfer in the structure shown in Fig. 1(a) is solved by an analytical model for near-field radiative transfer in one-dimensional structure, wherein the emitter and absorber include an arbitrary number of layers with the ith layer having thickness t_i and permittivity ε_i. The emitter is at uniform temperature T_e, and the planar absorber is at T_a, which is separated by vacuum gap d. The spectral thermal radiative flux across the gap can be calculated based on the energy exchange coefficient, ξ [63]

$$q(\omega) = \frac{\Theta(\omega, T_e) - \Theta(\omega, T_a)}{\pi^2} \int_0^\infty \xi(k_{//}, \omega) k_{//} dk_{//}. \quad (1)$$