Super-Planckian Thermophotovoltaics Without Vacuum Gaps

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(Received 6 June 2017; revised manuscript received 24 August 2017; published 9 November 2017)

We introduce the concept of a thermophotovoltaic system whose emitter is separated from the photovoltaic cell by an intermediate thick slab of gallium arsenide. Owing to the engineered structure of the emitter (a multilayer structure of negative- and positive-ε layers) together with a high refractive index and transparency of the intermediate slab, we achieve a super-Planckian and frequency-selective spectrum of radiative heat transfer which is desirable for the efficient performance of thermophotovoltaic systems.

DOI: 10.1103/PhysRevApplied.8.054020

I. INTRODUCTION

In the past two decades, many concepts for micron-gap and near-field thermophotovoltaic (NTPV) systems have been introduced [1–18] which have enabled the conversion of radiative waste heat into electric power by exploiting the photocurrent effect. Recently, NTPV systems in particular have been studied in great detail [4–18] because these systems can make use of the super-Planckian effect [19–23], which dramatically enhances the radiated power transferred from the emitter towards the photovoltaic (PV) cell and therefore could result in a large generated power. In this context, hyperbolic metamaterials [24] have received a great deal of attention [9,12,17] because of their beneficial properties allowing for large broadband heat fluxes and large propagation lengths [25–27]. However, NTPV systems suffer from many problems. One of the main problems is that it is necessary to maintain a vacuum gap between the emitter (which has a very high temperature) and the PV cell in order to have a super-Planckian effect, we need a material with a high refractive index so that modes which would be evanescent in vacuum could also contribute to the radiative heat transfer between the emitter and the PV cell. Second, the material must be highly transparent in the frequency band of operation to ensure that the bulk of the thermal radiation of the emitter is transferred towards the PV cell. Third, we need a material which has a relatively low thermal conductivity. This feature is necessary to limit the heat flux by electrons and phonons from the emitter to the PV cell in order to be able to keep the temperature difference between the emitter and the PV cell stable.

As a good candidate possessing these three features, we identify semi-insulating GaAs. It has a refractive index of about n ≈ 3.3 in the midinfrared regime [31] at which our device is operating. Furthermore, the absorption coefficient is negligibly low (approximately α = 0.01 cm⁻¹) for frequencies above 30 THz [31] that, for a 10-cm slab, more than 90% of the radiation is transmitted. The absorption by the phonons in GaAs is only meaningful for frequencies below 30 THz [31]. The absorption coefficient at very low frequencies can reach, e.g., α = 1 cm⁻¹, meaning that, for a 10-cm slab, the power would be completely absorbed by the slab. Finally, the last feature mentioned is related to the thermal conductivity of GaAs, which is approximately equal to κ ≈ 51 W m⁻¹ K⁻¹. However, the conductivity of GaAs is a function of the temperature, and the above value is given at room temperature (T = 300 K). If we assume that the emitter temperature is held fixed at 1000 K and the PV cell at 300 K, we can determine the amount of heat transported through the GaAs layer by Fourier’s law,

\[ Q = -\kappa \frac{dT}{dz}. \]  

II. ALTERNATIVE DESIGN OF FREE-GAP TPV SYSTEM

As can be seen from Fig. 1, we replace the vacuum gap between the emitter and the PV cell by a material which needs to have at least the following properties: First, in order to have a super-Planckian effect, we need a material with a high refractive index so that modes which would be evanescent in vacuum could also contribute to the radiative heat transfer between the emitter and the PV cell.
find the temperature profile \( T(z) = 0.6514(z/m) + 0.2042 \) K inside the GaAs film. We use this temperature profile to model the contribution to the radiated heat of the GaAs slab. The thermal power which is transported from the emitter towards the cell by heat conduction is then \( Q \approx 161.5 \) kW/m². This is a rather large value, but, as we show below, it is smaller than the purely radiative part.

In order to have an optimized radiative heat flow between the emitter and the cell, we optimize the emitter to match our PV cell, which is made of (In,As)Sb having a band-gap frequency of 65 THz. Therefore, we propose as emitter a multilayer structure made of tungsten (W) and germanium (Ge) layers modeling the relative permittivity of Ge as 17. The permittivity of W is taken from Ref. [32]. Here, we set \( d_m = 20 \) nm (thickness of the W layer) and \( d_d = 310 \) nm (thickness of the Ge layer). The whole emitter structure consists of only three periods of W/Ge layers on a tungsten substrate, as sketched in Fig. 1. The effective permittivity of such a multilayer structure is [24]

\[
\varepsilon_{\perp} = \frac{\varepsilon_m d_m + \varepsilon_d d_d}{d_m + d_d}, \quad \varepsilon_{||} = \frac{\varepsilon_m \varepsilon_d}{\varepsilon_m d_d + \varepsilon_d d_m} (d_m + d_d),
\]

where \( \varepsilon_m \) and \( \varepsilon_d \) are the permittivities of the tungsten and the germanium, respectively. In Eq. (2), \( \varepsilon_{\perp} \) represents the transversal component of the effective permittivity tensor (perpendicular to the optical axis), and \( \varepsilon_{||} \) is the longitudinal component (parallel to the optical axis). As Fig. 2 illustrates, \( \varepsilon_{\perp} \) is negative at frequencies below the epsilon-near-zero (ENZ) frequency. Therefore, the isofrequency surfaces of the metamaterial become hyperboloid at such frequencies so that the material has the properties of a type-II hyperbolic materials. For frequencies above the ENZ frequency, the isofrequency surface is an ellipsoid, so the emitter is effectively a normal uniaxial dielectric in that frequency range.

**III. NUMERICAL STUDY**

The thermal radiative power per unit area exchanged between the emitter and the cell is given by [33]

\[
S = \sum_{j=\text{p},s} \int_0^\infty \frac{d\omega}{2\pi} \int_0^\infty q \, dq \, P_{j}(\omega, q),
\]

where \( \omega \) represents the angular frequency, \( q \) is the spatial frequency, and \( P_{j}(\omega, q) \) is the spatial-frequency spectrum of radiative heat transfer corresponding to \( p \)- and \( s \)-polarized waves (power which is transferred per unit area to the PV cell per unit interval of frequencies \( \omega \) and unit interval of spatial frequencies \( q \)). Note that the
Planck’s mean energy of a harmonic oscillator \( \Theta(\omega, T) = \frac{\hbar \omega}{\exp(\hbar \omega / K_B T) - 1} \) \((K_B \text{ and } \hbar \text{ denote the Boltzmann and Planck constants, respectively})\) is included in the expression given for \( P(\omega, q) \). The transmission coefficient \( \tau_{p,s}(\omega, q) \) for \( p \) and \( s \) polarization can be extracted from \( P(\omega, q) \). There are several methods to determine \( P(\omega, q) \) exactly for multilayer systems \([33–36]\). Here, we use the equivalent-circuit model of Ref. [33]. Figure 3 shows the power spectrum with respect to the frequency which we obtain for our multilayer configuration. It can be seen that the radiative heat flux is, for most frequencies, much larger than that of two black bodies separated by a vacuum gap. Furthermore, we compare our exact results with the effective medium theory. Our results for the spectral heat flux obtained from the effective description in Fig. 3 suggest that the single resonance found in this case is connected to the high-energy transmission properties of hyperbolic materials at the ENZ frequency. However, when looking at the exact results for the power spectrum, we find three resonances, and the corresponding frequencies are the same for both \( p \) and \( s \) polarizations. To understand the underlying mechanism of these resonances, we plot the transmission coefficients \( \tau_{p,s}(\omega, q) \) in Figs. 4(a) and 4(b). We note that we find three branches for which the transmission coefficient is large for both polarizations. These branches belong to the three waveguide modes of lowest energy in the Ge layers which are coupled across the thin tungsten layers resulting in the split into three branches. These modes repeat themselves for larger frequencies (twice as large, 3 times as large, etc.), thus proving the Fabry-Perot–like properties of these coupled waveguide modes. As can be seen in Fig. 4, at the frequencies 77, 88, and 103 THz, the slope of these modes \( d\omega / dq \) is small, so the “density of states” is very large at these frequencies, resulting in a large thermal radiation at exactly those frequencies which correspond to the resonances in the spectral heat flux in Fig. 3. However, for the \( s \) polarization, the \( q \) region for which \( d\omega / dq \approx 0 \) extends over a smaller region than for the \( p \) polarization, thereby explaining why the resonances in the power spectrum are smaller for this polarization than those of the \( p \) polarization. It is worth noting that the transmission coefficient becomes zero after a certain value of the spatial frequency \( q_e = k_0 n \), where \( k_0 \) is the free-space wave number and \( n \) is the refractive index of GaAs) for each frequency. This is because the spatial frequencies higher than \( q_e \) correspond to the evanescent waves in the intermediate GaAs cavity, and hence these waves cannot contribute to the energy transfer over a distance of 10 cm.

Note that the resonances in the heat flux in Fig. 3 are spectrally located above the band-gap frequency of the PV cell, which is quite beneficial. Comparing the power spectrum with the blackbody radiation spectrum (the black curve), we achieve a sevenfold increase at the resonant frequency. This super-Planckian radiative heat transfer is expected to give a high output power for our PV cell. Using Eq. (3), the radiative power transferred into the PV cell is approximately equal to 225.2 kW/m\(^2\). Note that we also model the temperature gradient inside the GaAs layer and its contribution to the heat flux, which turns out to be
comparably small due to the large transparency of GaAs in the infrared. The radiative thermal power is compared to the thermal power due to the conduction in Fig. 5 for different temperatures of the emitter. As the temperature of the emitter decreases, the radiative heat transfer declines much faster than does the conductive heat transfer. However, for emitter temperatures larger than \( T_{\text{emitter}} = 915 \) K, the radiative heat becomes larger than the conductive heat, and it grows strikingly. At \( T_{\text{emitter}} = 1000 \) K, taking into account the conductive part of the heat transfer, the total thermal power transmitted between the emitter and the cell would be \( P_{\text{total}} = S + Q = 386.6 \) kW/m\(^2\). This value should definitely be lower than the maximum thermal power which can be removed by a water-cooling system [38]. As shown in our previous work [12], we can remove up to 390 kW/m\(^2\) with a water-cooling system. Therefore, we expect that the operation temperature of the PV cell can be easily kept at 300 K. However, it is worth mentioning that a portion of the power due to the radiative heat transfer is converted to electricity, and therefore the total thermal power which may cause an increase of the temperature of the PV cell is smaller than 386.6 kW/m\(^2\).

Let us now turn to the efficiency of our proposed TPV device. In general, the photovoltaic efficiency of the system is given by \( \eta_{\text{PV}} = \eta_{\text{OC}} \eta_{\text{QE}} \eta_{\text{FF}} \eta_{\text{UE}} \) [39]. The three first efficiency factors (open-circuit factor, mean quantum efficiency, and fill factor) depend on the intrinsic properties of the PV cell. To be able to make a more general statement, we focus on the ultimate efficiency \( \eta_{\text{UE}} \), which is associated with the power spectrum. It can be expressed as [39]

\[
\eta_{\text{UE}} = \frac{\int_{0}^{\infty} d\omega_{g} \omega_{g} dS}{\int_{0}^{\infty} d\omega dS},
\]

where \( \omega_{g} \) is the angular band-gap frequency. Since the power spectrum is narrow band and the resonances are located around the band-gap frequency of the PV cell, we can expect to have a large ultimate efficiency. Indeed, when calculating it for our device, we find \( \eta_{\text{UE}} = 52.2\% \). This value is high compared to the ultimate efficiencies obtained for the typical far-field TPV systems [39] (here, it is worthwhile to mention that, due to this fact and since these typical TPV systems with lower ultimate efficiencies and even higher emitter temperatures utilize a water-cooling system [39], our proposed water cooling system can also operate properly to maintain the temperature difference between the emitter and the PV cell of our TPV generator, which has higher ultimate efficiency). In our previous work [12], in which we designed a micron-gap thermophotovoltaic system using a hyperbolic medium.
(a wire medium), we also achieved about 50% ultimate efficiency. In that work [12], however, the super-Planckian radiative heat transfer was due to photon tunneling through a nanosize vacuum gap. Here, we achieve a similarly good efficiency without such a vacuum gap. The efficiency can be further improved by, for example, adding a filter on the PV cell which reflects the power beyond the band-gap frequency. However, in this paper, our target is to give a proof of concept for a thermophotovoltaic device using the near-field super-Planckian effect without having any vacuum gap. Optimization of the emitter-layer-cell structure can be done elsewhere. Nonetheless, it might be interesting to see how the ultimate efficiency and the total radiative power depend on the filling fraction of Ge in our narrow-band emitter. The results for both quantities are shown in Figs. 6(a) and 6(b) with respect to the thickness of the Ge layer while fixing the period of our multilayer structure at \(d_d + d_m = 330\) nm. For small thicknesses, the ultimate efficiency (about 40\%) is relatively small. For a \(d_d\) value close to 310 nm, a maximum efficiency of about 51\% occurs for the ultimate efficiency. For larger thicknesses, the ultimate efficiency drops to about 47\%. Therefore, our previous choice for \(d_d\) and \(d_m\) is already the best choice in terms of ultimate efficiency. As can be seen in Fig. 6(b), the radiative power is a monotonic function which increases as the \(d_d\) value does. Also, one might consider that an emitter with \(d_d = 320\) nm would give a better overall performance since the radiative power is, in this case, about 300 kW/m\(^2\), which is much larger than the 225.2 kW/m\(^2\) value found for our optimal device when \(d_d = 310\) nm. The problem in this case is simply that the total power transferred towards the cell by radiation and conduction is so high that the temperature of the PV cell can no longer be maintained at 300 K by a water-cooling system, thus making this configuration impractical.

### IV. CONCLUSIONS

In this paper, we introduce an alternative TPV concept which allows us to make use of the super-Planckian effect without the problematic necessity of maintaining a vacuum gap of a few nanometers between the emitter and the cell. The second advantage is that our device concept can be easily realized with existing nanofabrication methods. As shown theoretically, we achieve a large ultimate efficiency of more than 50\% together with large radiative heat fluxes of about 200 kW/m\(^2\) when choosing an optimized emitter design which allows for a narrow-band thermal emission around the band gap of the PV cell. We believe that our concept opens a route towards more practical and more realistic super-Planckian TPV systems without any vacuum gaps.

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[38] G. Mattarolo, Development and Modelling of a TPV System (University of Kassel Press, Kassel, Germany, 2007).