Light-trapping in photon enhanced thermionic emitters

Jeronimo Buencuerpo,1 José M. Llorens,1,2 Pierfrancesco Zilio,2 Waseem Raja,2 Joao Cunha,3 Alessandro Alabastri,2 Remo Proietti Zaccaria,2 Antonio Martí,4 and Thijs Versloot3

1IMM-Instituto de Microelectrónica de Madrid (CNM-CSIC), Isaac Newton 8, PTM, E-28760 Tres Cantos, Madrid, Spain
2Istituto Italiano di Tecnologia, via Morego 30, 16163 Genova, Italy
3Advanced Concepts Team, European Space Research and Technology Centre, Noordwijk, The Netherlands
4Instituto de Energía Solar, Universidad Politécnica de Madrid, ETSI Telecomunicacion, Ciudad Universitaria sn, Madrid 28040, Spain

Abstract: A series of photonic crystal structures are optimized for a photon enhanced thermionic emitter. With realistic parameter values to describe a p-type GaAs device we find an efficiency above 10%. The light-trapping structures increases the performance by 2% over an optimal bilayer anti-reflective coating. We find a device efficiency very close to the case of a Lambertian absorber, but below its maximum performance. To prevent an efficiency below 10% the vacuum gap must be dimensioned according to the concentration factor of the solar irradiance.

References and links

1. Introduction

Power generating devices operating in extreme conditions are of great interest for pushing the current exploration limits in the solar system. An illustrative and highly challenging example is harvesting solar energy in a near Sun orbit. The upcoming European Space Agency’s Bepi Colombo mission to Mercury (0.30–0.47 AU) [1] will be exposed to high-energy particle fields and light intensities of up to 10.6 suns, resulting in operating temperatures as high as 500 K. Standard space photovoltaic solar cell systems however exhibit degraded performance above a maximum steady-state operating temperatures of 420 K. For the future, even closer observation missions are planned [2], with ESA’s Solar Orbiter at 0.28 AU and NASA’s Solar Probe Plus set to perform multiple close approaches at 0.04 AU. At this distance, the face temperature can easily reach as high as 1700 K. In both concepts, specially screened photovoltaics are foreseen to be used during the outer part of the orbit trajectories, where the heat flux is considered manageable. Key to enhance mission performance is therefore to extend the capability to higher operating temperatures. In this study, we propose the use of a photon-enhanced thermionic emitter (PETE) [3] as an alternative to conventional solar cells with the capability to operate in a temperature range beyond 500 K.

In its original conception [4], a thermionic energy converter (TEC) operates as a thermoelectric device where a vacuum gap is introduced to preserve the temperature difference between the hot and cold terminals (see Chap. 13 of [5] for a historical review). The material removal has a detrimental impact on the current crossing the device given that the electrons must be emitted from the cathode to the anode instead of relying on the conventional drift and diffusion mechanisms and an electrostatic potential build-up by the emitted electrons in the gap. Depending on materials, a practical TEC requires emitter temperatures in the range 1600–2000 K [6].

In the PETE design, Schwede et al. proposed to use a cathode comprising a semiconductor in order to increase the conduction band population through photon absorption [3]. In this way, the performance could be enhanced at lower temperatures by optimally combining thermal and photovoltaic processes. Fundamentally, the maximum attainable efficiency converges to the efficiency of a solar thermal converter and can surpass 60% at a concentration of 1000 suns [7]. Very recently the efficiency limit has been reviewed by Segev et al. in [8] taking as a reference the Shockley-Queisser (SQ) limit [9]. The efficiency of an isothermal operating PETE device, can be described as a Metal Insulator Semiconductor (MIS) solar cell [10] which is bounded by the SQ limit. A PETE might exceed both the SQ limit and the ideal thermal limit if operated non-isothermally at high temperatures. However, Segev et al. recognize that the optimal operating temperatures largely exceeds the limiting temperature of actual semiconductor devices.

In this study, we discuss the feasibility of achieving a high efficiency PETE in the intermittent temperature range of 500–800 K. We concentrate our effort in providing an optimized cathode structure integrating photon absorption, carrier transport and surface emission. The photon absorption is enhanced with the help of a front light-trapping structure (LTS) based on a periodic photonic crystal. As cathode material we have considered GaAs, which is a reference material in solar cell technology. Even though other materials might perform better than GaAs at higher temperatures (e.g. GaN) their optical properties are not that well characterized as a function of the temperature, a critical element in the design of an LTS. In addition, GaAs exhibits excellent technological advantages, like ultra-low surface recombination velocity at the GaAs/GaInP interface [11] and therefore has been used in recent experimental realizations of PETE devices [12, 13]. We have explored four different structures combining dielectric cones and cylinders. The structures are optimized using a device model with a 1D electronic diffusion model [14, 15] adapted for an arbitrary generation profile. A semi-analytical approach is taken which allows on an efficient calculation of the PETE performance in the optimization
procedure. For comparison, we made use of two ideal physical systems: a Lambertian absorber and a single pass Beer-Lambert absorber. They constitute the upper and lower limits in terms of light absorbed without reflection losses, respectively. The maximum efficiency expected for a GaAs based PETE operating at 700 K is close to 16% for a Lambertian-like cathode of ~30 nm. In a realistic PETE with a light-trapping structure this value reduces to 11% to 12% and the thickness increases to ~225 nm. We find that the distance to the Sun, or equivalently, the concentration factor is critical in determining the dimensions of the vacuum gap. If it is larger than 10 μm, the PETE efficiency is smaller than 10% at a concentration of 100 suns. A larger vacuum gap would require a lower concentration factor to not quench its performance.

2. Physical model

The PETE device consists of a p-type semiconductor hot cathode and a cold metal anode. The light impinges at the front surface (transmission configuration, [17]) and the photogenerated electrons diffuse towards the back surface where subsequently the emission takes place. In this study, a light-trapping structure is positioned at the front surface. Figure 1 shows a scheme of the different parts of the device. Contrary to conventional solar cells, it is not possible to enhance the absorption in the cathode by placing a mirror at the back surface, because it would complicate the thermionic emission process. For efficient emission, the semiconductor should have low electron-affinity (ϕ), or alternatively, its surface should be subjected to a Cs treatment [18]. As a final process, the emitted electron will create a electrostatic potential in the vacuum region. In summary, the physical model consists of four different elements: (i) first to compute the photon absorption along the cathode; (ii) to determine the generation rate from absorbed light; (iii) to calculate the carrier concentration at the emission surface and the emitted current; (iv) to compute the electrostatic barrier height in order to get the net emitted current. In the current study we have not considered the heat balance between the Sun and an eventual PETE panel as we want to identify the optimal operational conditions of the device. As any service module in a satellite, its optimal temperature range of operation would be granted through a thermal management system which would emit or retain the heat radiation as a function of the orbit position and orientation with respect to the Sun or a near planet.

2.1. Optical absorption

The optical absorption is computed by means of the Fourier Modal Method (FMM). In this method the electromagnetic fields are expanded on an eigenmode basis. The structure is approximated by slices of constant refractive index along the propagation direction. On each slice a scattering matrix is defined that relates all the incoming channels with the outgoing channels. Combining the different scattering matrices allows to determine the scattering matrix of the full stack. This work uses the implementation of the method found in the open source software S4 [19].

2.2. Transport model

A full description of the PETE transport model would require a 3D description of the generation process and drift-diffusion of the photogenerated carriers. This is a highly computationally demanding task. Andreani et al. have shown that to a great extent the device can be approximated by averaging the generation in the normal plane to the electron propagation direction [20]. In addition, finite-element-method simulations have also shown that the drift transport can be safely neglected in the range of voltages meaningful for the PETE [21]. To model the charge transport in the device, we have implemented the 1D diffusion model developed by Varpula and Prunilla [14]. The net current density results of the sum of the cathode and anode currents
Fig. 1. Depiction of the different parts of a PETE device. Light impinges from the left side on the light-trapping structure. The band structure of the cathode and anode is depicted for a voltage at the flat-band condition. The red curve in the vacuum gap represents the charge-cloud electrostatic potential.

\[ J = J_C - J_A. \]

The current densities are described by the Richardson-Dushman equations [3]:

\[ J_C = A_C T_C^2 \exp \left( -\frac{\Delta E_C}{k_B T_C} \right) \frac{n}{n_{eq}}, \]

\[ \Delta E_C = \phi_C + \Theta(V - V_{fb})(V - V_{fb}), \]

where \( A_C \) the Richardson constant, \( T_C \) the cathode temperature, \( k_B \) the Boltzmann constant, \( n \) the electron density at the emission surface, \( n_{eq} \) the electron density at equilibrium, \( \phi_C \) the cathode work function and \( \Theta(x) \) the Heaviside function. The work function is defined in terms of the electron affinity \( \chi_C \), conduction band edge \( E_C \) and Fermi energy \( E_F \) as \( \phi_C = E_C - E_F + \chi_C \). The flat-band voltage is defined by the alignment of the cathode and anode work functions:

\[ V_{fb} = (\phi_C - \phi_A)/e. \]

A similar expression to Eq. (1) is derived for the anode:

\[ J_A = A_A T_A^2 \exp \left( -\frac{\Delta E_A}{k_B T_A} \right), \]

\[ \Delta E_A = \phi_A + \Theta(V_{fb} - V)(V_{fb} - V). \]

Note that the expression of \( J_A \) corresponds to a pure thermionic emission and therefore the electron density is absent.

The electron density can be divided into two contributions, the electron density at equilibrium and the photogenerated electrons:

\[ n(x) = n_{eq} + \Delta n(x). \]

The diffusion law governing the electron transport can be expressed as [14]

\[ D \frac{d^2 \Delta n}{dx^2} = \frac{\Delta n}{\tau} - G(x), \]

where \( D \) is the diffusion constant of the electrons, \( \tau \) is the electron lifetime and \( G(x) \) is the generation rate. A popular approach taken in the literature is to assume the generation created by the absorption of light following the Beer-Lambert law [14, 15, 17, 22]. In our case, the generation is computed from the x-component of the Poynting vector integrated over the area of the photonic crystal unit cell (\( S_x \)) obtained from the FMM:

\[ G(x) = \int_{E_x}^{\infty} dE \frac{\Phi_{AM0}}{E} \left( -\frac{1}{S_0} \frac{dS_x}{dx} \right), \]
where $E_g$ is the cathode bandgap, $S_0$ is the normalization flux considered in the FMM calculation and $\Phi_{AM0}$ is the zero air mass solar spectral irradiance. The solution of Eq. (4) is found after imposing the boundary conditions at the front and back surfaces:

$$\frac{d\Delta n}{dx} \bigg|_{x=0} = \frac{R_{S0}}{D} \Delta n(0),$$

$$\frac{d\Delta n}{dx} \bigg|_{x=W} = -\frac{R_{SW}}{D} \Delta n(W) - \frac{J}{qD},$$

where $R_{S0}$ and $R_{SW}$ are the surface recombination velocities of the front and back surfaces. The total current appears in the back boundary condition, meaning that there is a closed loop dependence between the excess carrier density and the net emitted current. The system of equations as formulated above is a boundary value problem (BVP) solvable with a mathematical symbolic software [23]. The integral of $G(x)$ in the cathode region is the only step required to evaluate numerically. However, under high injection conditions ($\Delta n/p > 1$) the electron lifetime cannot be assumed to be constant and its explicit dependence on radiative and Auger recombination processes therefore needs to be introduced in Eq. (3) thus resulting in a non-analytic BVP [15]. Although the numerical solution can be easily found nowadays, the increase in computational time makes the optimization procedure highly demanding. In this study the low injection condition is satisfied as can be seen in Fig. 5, where $n < N_A$.

2.3. Space charge model

The charge cloud created by the emitted electrons cannot be straightforwardly implemented in Eq. (3). Instead, we have independently solved the Poisson’s equation to obtain the maximum of the electrostatic potential ($\phi_e$) taking as starting point the saturation current ($J$ at $V < V_{FB}$) [6, 16]. Finally, we introduce $\phi_e$ in $AE_C$ in Eq. (1) to recompute the $JV$ curve introducing the reduction in the probability of emission due to the charge cloud. We will further develop this point in section 3.4.

2.4. Candidates to light-trapping structures

It has been already mentioned that we will rely on photonic structures to enhance the absorption in the cathode. In this way, a PETE with a thinner cathode can be obtained to minimize transport losses without sacrificing a loss in absorption. The front material considered in the simulations is SiO$_2$, given that the PETE device needs to be encapsulated to get protected from the outer space. We have explored the performance of four different structures. We show a sketch of the different elements and materials defining each of the structures in Fig. 2.

A GaAs slab, as cathode, finished by an anti-reflective coating made of a bilayer (structure S0 in Fig. 2) will serve as a reference of the state-of-the-art technology employed in space for conventional solar cells. The other three structures include a photonic crystal of lattice parameter $a$. This photonic crystal contains two well differentiated layers. The top layer is common to all structures. It contains a dielectric cone of radius $R$ and height $h$; a Moth-eye like structure which is well known to reduce the reflectance by reducing the refractive index mismatch between the SiO$_2$ cover and the GaAs cathode [24–29]. The bottom layer characteristic of each structure. In the structure S1, a dielectric (TiO$_2$) cylinder is placed below the top cone. Its presence is justified because this structure might help in increasing the diffraction efficiency of higher diffractive orders, which are characterized by larger optical paths and hence a higher absorption in the cathode. In structure S2, the dielectric cylinder is substituted by a dielectric slab. We have seen in previous studies that a thin slab helps in coupling light to guided modes, which again will result in a higher absorption of the Sun light [29]. One problem of the structures S1
and S2 is the small refractive index contrast between TiO$_2$ and SiO$_2$. In general, the higher the contrast, the higher the diffraction effects. Therefore, we have considered structure S3, which is similar to S2, but the TiO$_2$ cylinder is substituted by a GaAs cylinder. In this structure, we are increasing the surface of the active device and therefore its surface recombination will be higher than in the case of the other structures. An additional shortcoming is that our 1D model can not accurately describe the transport along the cylinder. For this structure we have assumed that the cathode thickness is $d + W$ instead of just $W$.

3. Results and discussion

3.1. Light-trapping structures optimization

The four photonic structures are optimized under the same conditions, using a global optimizer \cite{30,31} and the power ratio as figure of merit:

$$\eta^* = \frac{J(V_{op})V_{op}}{P_{inc}}$$

being $V_{op}$ the operation voltage where the PETE delivers maximum power output and $P_{inc}$ is the incoming solar irradiance.

Table 1. Parameters and conditions used in the optimization. Parameters marked as $^\dagger$ are extracted from \cite{32}

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D^\dagger$</td>
<td>200 cm$^2$/s</td>
<td>$m_a^\dagger$</td>
<td>0.067 m$_e$</td>
<td>$\phi_d$</td>
<td>0.9 eV</td>
</tr>
<tr>
<td>$R_{so}$</td>
<td>100 cm/s</td>
<td>$m_p^\dagger$</td>
<td>0.47 m$_e$</td>
<td>$\tau$</td>
<td>0.4 eV</td>
</tr>
<tr>
<td>$R_{sw}$</td>
<td>1 cm/s</td>
<td>$\alpha_C$</td>
<td>120 m$_n = 8.04$ A cm$^2$</td>
<td>$T_C$</td>
<td>700 K</td>
</tr>
<tr>
<td>$N_A$</td>
<td>$10^{18}$ cm$^{-3}$</td>
<td>$\alpha_A$</td>
<td>120 A cm$^2$</td>
<td>$T_A$</td>
<td>573.15 K</td>
</tr>
<tr>
<td>$\tau^\dagger$</td>
<td>5 ns</td>
<td>$X$</td>
<td>100 suns</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The parameters defining the operating conditions of the PETE that we use in the optimization can be found in Table 1. To keep the model semi-analytic the lifetime and diffusion coefficients are kept constant in solving the output current. The surface recombination velocity at $x = 0$ is set to 100 cm/s, which could be achieved using back surface field (BSF) \cite{10,21}. On the other hand, the recombination surface at $x = W$ is taken as 0 cm/s, to illustrate that the emission rate dominates over the surface recombination. The anode temperature, $T_A$, is set to 573.15 K. Keeping the anode at a high temperature may allow to introduce an auxiliary Carnot machine.
to increase the final PETE efficiency [3]. A thorough analysis of the PETE performance for different values of $\chi$, $N_A$, and $X$ is reported in [14, 15]. In our study, we will take as realistic values $\chi = 0.4$ eV, $N_A = 10^{18}$ cm$^{-3}$ and $X = 100$ suns. The latter might represent either the increase of the solar irradiance in a near Sun orbit or an optical concentration system or a combination of both. The cathode temperature is kept fixed at 700 K if not said otherwise. Later, the effect of the temperature will be analyzed between 350 K and 1000 K. We have verified by a simple thermal energy balance that this temperatures might be achieved at $X = 100$ suns. Similarly to [22] we have considered as source the incoming solar flux and as drain the work used to extract the electrons form the cathode, the radiation losses (assuming the cathode as black-body at temperature $T_C$ with emissivity from $E_g$ to higher energies, $P_0$) and an additional ideal IR coupler (also a black-body but with emissivity up to $E_g$, $P_{IR}$):

$$P_{mc} - J[\phi C + (V_{op} - V_{fb})/(V_{op} - V_{fb})] = P_0 + P_{IR}.$$  \hspace{1cm} (7)

The equilibrium temperatures are 1000 K and 1100 K if the IR coupler is present or absent, respectively. Hence, the analysis shows that the solar flux provides enough power to cover the temperature range of our study.

The optimization of the size parameters corresponding to each structure is bounded between the following limits. The lattice parameters vary between 100 nm to 1 $\mu$m. The filling factor, defined as the ratio between the diameter of the cylinder and the lattice parameter, varies between 0.25 to 1. The height of the cone and cylinder share the same bounds between 0 $\mu$m to 1 $\mu$m. The cathode thickness is bounded between 1 nm to 20 microns. Finally, the spectral range chosen in the optimization spans from 1 eV to 4 eV, i.e. 310 nm to 1240 nm. It covers 80% of the solar irradiance AM0. The other 20% distributes as 1% at higher energies and 19% at lower energies. The lower energy contribution of the solar irradiation can not be directly absorbed by the semiconductor, therefore it has been proposed to use an infra-red filter as a heating system. The higher energy contribution can be absorbed by the semiconductor, but as we will see, at such high energies also the dielectrics compete in absorption. Once the upper and lower bounds are set, the optimizer evaluates directly $\eta^*$ under the operating conditions defined in Table 1. The optimal parameters found by the optimizer are shown in Table 2 together with the $\eta^*$ value. In addition, we have introduced the corresponding value of the ultimate efficiency $\eta_{ue}$ [9]. This figure of merit is very popular in the design of optical coatings for conventional solar cells and it will serve to highlight the particularities of the PETE optimization.

<table>
<thead>
<tr>
<th>System</th>
<th>$a$ (nm)</th>
<th>$R$ (nm)</th>
<th>$h$ (nm)</th>
<th>$d$ (nm)</th>
<th>$W$ (nm)</th>
<th>$\eta^*$</th>
<th>$\eta_{ue}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>S0</td>
<td>-</td>
<td>-</td>
<td>67.1</td>
<td>43.8</td>
<td>348</td>
<td>10.12</td>
<td>33.35</td>
</tr>
<tr>
<td>S1</td>
<td>584</td>
<td>292</td>
<td>814</td>
<td>21.7</td>
<td>224</td>
<td>11.48</td>
<td>34.97</td>
</tr>
<tr>
<td>S2</td>
<td>612</td>
<td>292</td>
<td>847</td>
<td>27.2</td>
<td>220</td>
<td>11.72</td>
<td>35.57</td>
</tr>
<tr>
<td>S3</td>
<td>387</td>
<td>147</td>
<td>123</td>
<td>209</td>
<td>28.4</td>
<td>12.43</td>
<td>38.25</td>
</tr>
</tbody>
</table>

As expected, Table 2 reveals that the introduction of a photonic crystal results in an increase of the PETE efficiency with respect to the bilayer structure, which constitutes the state-of-the-art in terms of optical coating. Structures S1 and S2 exhibit a very similar performance. Their size parameters are also very close in value, with a slightly larger lattice constant for S2. The absence of a cylinder as scatterer in S2 leads to a weaker diffraction, which is compensated by a larger lattice constant and a taller cone. Structure S3 brings remarkable differences with respect to structures S1 and S2. The lattice constant and filling factor are significantly smaller, a reduction of $\sim 35\%$ and $\sim 50\%$, respectively. This reflects that S3 mostly operates in the sub-
We show in Fig. 3 the optical absorption of the different structures. From a qualitative point of view, it is possible to recognize the diffractive character of S1 and S2, where the spectrum shows sharp resonances at low energies. The S3 spectrum, instead, shows more smooth peaks typical of sub-wavelength structures. The ultimate efficiency $\eta_{ue}$ results very helpful in comparing the absorption performance of each structure. From Table 2, there is a clear correlation between the $\eta^*$ and $\eta_{ue}$, hence the higher the absorption, the higher the PETE efficiency. However, if we keep all the size parameters constant and let grow $d$ and/or $W$, $\eta_{ue}$ keeps increasing up to its maximum theoretical value ($\eta_{ue,max} = 43.5\%$), while $\eta^*$ reduces monotonously. The optimization of $\eta^*$ takes into account the loss of electrons in the diffusion process across the cathode. A further analysis of Fig. 3 permits to quantify the amount of light absorbed by the TiO$_2$. The dashed vertical line indicates the TiO$_2$ band edge. The dashed colored lines represent the absorption for a lossless TiO$_2$. Hence, the losses in the dielectric are the hatched areas. The losses are more critical in S1, and S2, whereas S3 does not present this problem. In our case the TiO$_2$ refractive index were temperature independent, therefore it is expected that the band-edge would red shift in a real device. We can conclude that S3 is the best solution as light-trapping structure as long as a dielectric of larger bandgap than TiO$_2$ at equal refractive index is not available.
3.2. Effect of the cathode thickness and temperature

The S0 structure strategy to enhance the absorption is to minimize the reflection losses. Structures S1 to S3 strategy is two-fold. It consists in reducing the reflection losses together with increasing the optical path. The physical grounds of these two strategies can be represented by two different ideal physical models [35]:

- A single pass Beer-Lambert absorber (BLA) without reflection. The Poynting vector in a BLA is defined as:

\[ S(x)_{\text{BLA}} = \exp[-\alpha(E) x], \]

where \( \alpha(E) \) is the absorption coefficient.

- A Lambertian absorber (LA), also without reflection. For an LA, the Poynting vector is:

\[ S(x)_{\text{LA}} = \frac{1}{4\pi^2 \alpha(E)x + 1}. \]

The evolution of \( \eta^* \) with the cathode thickness is shown in Fig. 4(a). We have kept fixed all size parameters except \( W \). For the structure S3, we have assumed as cathode thickness the sum \( d + W \), but keeping the same ratio \( d/W \) as in the case of the optimal structure of Table 2. The efficiency of S0 increases with \( W \) up to a thickness of \( \approx 350 \) nm. For thicker cathodes the efficiency drops. The good agreement between S0 and BLA indicates that the absorption increases in the cathode up to a thickness where all the incoming light gets absorbed. For larger values of \( W \) there is no additional generation and the loss mechanisms in transport are responsible of the efficiency drop. The shoulder appearing at \( \approx 25 \) nm is related with the zero-frequency Fabry-Perot mode [36], meaning a resonance peak. The efficiency of S1 and S2 follows a very similar trend. As expected, the dielectric photonic crystal structure helps in increasing the absorption in the cathode reaching a clear maximum at the optimal \( W \). For these structures it is also possible to identify the zero-frequency at \( \approx 25 \) nm. Structure S3 only
outperforms S1 and S2 in the neighborhood of the optimal $W$. This is attributed to its design. S1 and S2 with a thinner cathode keep the same dielectric photonic crystals. However, the cathode thickness in S3 is $d + W$, hence the height of the cylinder in the S3 structure varies and the diffracting structure reduces the light-trapping. The LA efficiency is above all structures and can be considered as a top physical limit. It exhibits a maximum for thinner cathodes as the absorbed power saturates "faster" than in BLA and the realistic structures. The fact that maximum efficiency of S3 gets very close to the LA efficiency shows the good performance of the structure as anti-reflective coating. This is a known behavior of photonic crystals based on cones [26–29]. Finally, for $W > 1 \mu m$ all models converge and follow the same trend.

In Fig. 4(b), we show the evolution of the efficiency with the cathode temperature. The shape of the curves is similar for all the structures. At low temperatures the efficiency is low because the electrons do not have enough energy to overcome the escaping barrier, ($\Delta E_C$ in Eq. 1) and the reverse current from the anode (at $T_C = 573$ K) dominates. At higher $T_C$, the efficiency grows exponentially in accordance with $J_C$ up to maximum value. From this point, the generation process is not powerful enough to keep a high current and only the LA keeps increasing with $T_C$. Only at very high temperatures (higher than 900 K) the $n_{eq}$ is high enough to allow the electrons to escape from the cathode ("purely" thermionic emission). Structures S0-S3 and BLA show a reduction in efficiency attributed to the drop in voltage. The bandgap of the semiconductor reduces with the temperature and consequently the voltage at flat-band gets also reduced. We will come back to this point when discussing the internal operation of the PETE in Fig. 5.

To get a full understanding of the efficiency of the PETE it is customary to look at the evolution of the internal variables of the device namely the operation current density and voltage and the carrier density at the emission surface. We have constrained this analysis to the two physical models BLA and LA, as the actual structures exhibit an "in-between" behavior. The evolution of the current density follows qualitatively the same trends as the efficiency, therefore we have omitted the corresponding plots. The evolution of the voltage with $T_C$ was analyzed in [15]. We show the results for the BLA and the LA in Fig. 5(b). Naively thinking, the operating voltage
3.3. Refractive index temperature dependence

One of the key material parameters of our study is the permittivity or, equivalently, the refractive index. GaAs is one of the few semiconductor materials thoroughly studied from an optical point of view in a broad temperature range. Its optical response is characterized by a series of high absorption peaks, related with the Van Hove singularities of its electronic band structure [37]. The impact of the temperature on the refractive index is a red shift of the resonances positions.
and an increase of their spectral width. An ab-initio calculation of the linear response as a function of the temperature still represents a computational challenge [38,39] out of the scope of the present work. Nevertheless, it is possible to get an accurate description relying on a simple empirical model [40]. We have neglected the impact of excitonic effects in our analysis, given that we are targeting very high temperatures. In Figure 6, we show the evolution of the real and imaginary part of the refractive index within a temperature range of 300 K to 1000 K. The most noticeable changes in the spectral range of interest is the red shift of the fundamental bandgap (Γ point, $E_0$ transition) and the absorption along the Γ-L line ($\Lambda$ line, $E'_0$ transition). At higher energies there are two additional transitions $E_2$ (X point) and $E'_0$ (excited conduction band at the $T$ point).

The change in the absorption spectrum of the optimal structures is depicted in Fig. 7(a)-(c). We have not shown the corresponding spectra of structure S1, because qualitatively it is similar to that of S2. It is common to all structures the red shift of the fundamental bandgap. In fact, the increase in broadening and value of $\text{Im}(n)$ gets reflected as the increase in the absorption with the temperature in the low energy part of the spectrum. The rise of $\text{Im}(n)$ at high energies ($E_2$ and $E'_0$ transitions) is hindered by the absorption of the TiO$_2$, which starts to absorb from 3.2 eV onwards, as discussed above. The general trend is therefore a rise of the absorbed light with temperature for energies below 2.5 eV and an almost insensitive absorption for higher energies. The effect of the temperature on the absorption can be quantified by looking at the ultimate efficiency ($\eta_{ue}$). Fig. 7(c) shows the corresponding values for each of the structures. It is clearly identifiable the increase in $\eta_{ue}$, directly related with the absorption, in all structures. While the bilayer structure (S0) shows a linear-like increase with the temperature, S1 and S2 show step changes in slope. This is related with the excitation of resonances appearing at low energies [Fig. 7(b)]. The behavior of structure S3 instead shows a clear maximum at 800 K, very close to the temperature used in the optimization, 700 K (see Table. 1). Hence, the evolution of the refractive index with the temperature needs to be taken into account explicitly to get an

![Absorption Spectra](image)

Fig. 7. Change in the optical absorption as a function of the temperature for the optimal structures S0 (a), S2 (b) and S3 (c) defined in Table 2. The dependence of the complex refractive index is depicted in Fig. 6. The color gradient from red to blue corresponds a temperature gradient from 300 K to 1000 K. (d) The ultimate efficiency as a function of the temperature for the optimized structures (S0 gray line, S1 blue line, S2 red line and S3 black line).
accurate description of the optical absorption. Alternatively, one could have taken the refractive index at 300 K and shift it according to the fundamental band-edge. Such approach would imply an underestimation of the total absorbed light.

3.4. Charge-cloud effects

In an ideal PETE device, the totality of the emitted electrons from the cathode will reach the anode and vice versa. However, as it has been already mentioned, the vacuum gap is not a ballistic channel for the emitted electrons. Intuitively, emitted electrons will interact electrostatically with one another. The result is that some of the electrons reflect back to the cathode. Depending on the applied voltage, there is a point in the space between cathode and anode of maximum probability of backscattering in the steady state. Such maximum has been depicted in the energy level structure of Figure 1 by the electrostatic potential maximum $\phi_e$. Beyond this point, the electrons reach the anode ballistically. A rigorous description of this problem is based on the Langmuir space charge theory [41], which has been successfully adapted to the case of thermionic emitters [6] and PETE [16]. The value of the applied voltage plays a critical role in the final profile of the electrostatic potential and three regimes are clearly identified: (i) Saturation point: the voltage $V_s$ is such that $\phi_C > \phi_A$ and $\phi_e$ is located within the cathode physical space; (ii) Critical point: the opposed situation, the voltage $V_C$ is such that $\phi_C < \phi_A$ and $\phi_e$ is located within the anode physical space; (iii) Space charge limited regime: this is the “in-between” regime depicted by the red line of Figure 1. We have followed the numerical procedure described in [6, 16] to determine the value of $\phi_e$ as a function of the voltage given a certain saturation current and a vacuum gap distance. However, they assumed in their work that the operating current density in the space charge limited regime is $J(V) = J_C \exp[-\phi_e(V)]$, which is valid for a thermionic emitter but only an approximation for PETE. We showed in Eq. (1) that the current density depends on the electron concentration $n$ and in Eq. (5) that $\Delta n$ also depends on the current density. The solution of this system of equations would require a self-consistent solution scheme at each value of the voltage. Instead, we have adopted an approximate solution. We first calculate the saturation current $J_C$ as described in Section 2. The potential barrier $\phi_e(V)$ is calculated only once for this maximum current density supplied by the PETE. Then, we introduce $\phi_e(V)$ in the exponential of the current density [$\Delta E_C$ in Eq. (1)] and recompute the $JV$ curve.
We show in Figure 8(a) the change in the characteristic $JV$ curve of the S3 PETE as a function of the vacuum gap distance and in Figure 8(b) the corresponding value of $\phi_e$. In the limit of zero vacuum gap, the $JV$ curve is exactly the same to the ideal PETE, all the emitted electrons reach the anode seamlessly. The drop in current takes place close to the flat-band voltage (indicated by the vertical line for $\phi_e = 0$). For this vacuum gap $V_S \approx V_C \approx V_0$, and $\phi_e \approx 0$. When the vacuum gap distance increases, the drop in the current density takes place at lower voltages, mostly governed by the value of the saturation voltage $V_S$. The barrier $\phi_e$ starts to increase accordingly. To get a broad picture on the impact of $\phi_e$ on the performance of the device, we have depicted in Figure 8(c) the evolution of the PETE efficiency with the vacuum gap distance. The reduction in efficiency at a concentration of 100 suns (default conditions) is very slow for a very thin gap, from 0 $\mu$m to 3 $\mu$m. For wider gaps, the drop follows an almost linear decrease. This effect is tightly related with the amount of photogenerated and emitted electrons. Therefore changes in the concentration factor have a great impact on the performance of the device. Higher concentrations produce higher current densities and, in accordance, faster reductions in performance with the vacuum gap distance (see blue line for 1000 suns). The opposite behavior is found for lower concentration factors. It is possible to keep a constant performance up to 25 $\mu$m gap for 10 suns. The technology employed in the fabrication of the PETE device would critically determine the optimal concentration factor to avoid sacrificing the performance of the device. For sub-micrometer to a few micrometers gap, high concentration provides the best performance. For technology involving larger fabrication motives a low concentration factor is mandatory. In contrast to TECs, where $T_e \neq T_a$, a PETE can operate in an isothermal configuration. Thus, a narrow vacuum gap would not be affected by the near field heat exchange [37].

4. Conclusions and outlook

The description of a PETE with a light-trapping structure required a model able to cope with an arbitrary generation profile and a full description of the complex refractive index as a function of the temperature. We have focused our analysis on two parameters only, the cathode thickness and its temperature. The photonic crystal structures provides an $\approx 12\%$ efficiency at thicknesses around $\approx 225$ nm. This value is very close to the physically ideal system of non-reflective Lambertian absorber. There is still place of improvement, given that a $16\%$ efficiency might be achieved for a very thin absorber ($\approx 25$ nm). Further research is required to achieve such value. At low temperatures, the PETE offers a maximum performance at smaller temperatures than the anode ($\approx 525$ K and 573 K, respectively). As reported in [3, 15, 21], a higher efficiency is attainable by heating up the cathode beyond 1000 K. However, such temperature regime is far beyond of the operational temperature limit of semiconductor devices. The role of the charge cloud created by the emitted electrons also plays a strong constrain on reaching an efficiency above 10%. We found that the concentration factor is critical in determining the optimal vacuum gap distance. Keeping it bellow 100 suns allows for a vacuum gap narrower than 10 $\mu$m, while higher values required much narrower channels.

The efficiency values reported here are greater than those of a single junction GaAs solar cell in the SQ limit at temperatures above $\approx 1000$ K. Clearly, the combination of photovoltaic and thermal conversions is critical for the PETE to outperform a standard solar cell. However, such crossover needs to be moved to lower temperatures for practical applications to be attractive. At the same time, it offers technological advantages. The extraction of electrons and holes can be done selectively and no p-n junction is required [21, 42]. This prevents problems related with the migration of dopants and the removal of the built-in voltage for carrier separation. Problems related with the diffusion of contacts are common to solar cells and PETEs. A feasible way to enhance the efficiency of the PETE is to rely on semiconductors of broader bandgap. Indeed, the optimal bandgap is around 1.4 eV [3]. An additional benefit is the increase of the effective mass
with the bandgap providing higher values of the Richardson-Dushman constant $A'$. However, the electron-affinity also increases with the bandgap, requiring a more effective Cs treatment.

In terms of space applications, the reported PETE shows to be competitive with existing technology when targeting high intensity solar radiation and high temperatures. Even though previous tests [43] reported concentrator cells with 18% of AM0 efficiency surviving 7 minutes at 870 K, solar cells show a substantial decrease in efficiency above 370 K. For example, typical InGaP/GaAs/Ge triple junction solar cells with efficiency $\eta = 26\%$ at $T = 300$ K and with linear normalized temperature coefficient $\beta = (1/\eta)(d\eta/dT) = -4.5 \times 10^{-3}$ K$^{-1}$ [44] are expected to have an efficiency of 11% at 420 K (average temperature orbiting Mercury under a solar concentration factor of ~ 10 suns [1]). At 440 K the efficiency is already below 10%. Single junction GaAs on Ge solar cells with lower $\beta$ show a drop of efficiency from 17.6% (300 K) to 14% (420 K) [43] and for $T = 530$ K and higher, besides the poor thermal stability of the system, the efficiency drops off below 10% resulting in decreased performance. A PETE system working at 10% efficiency would therefore be advantageous above temperatures of 570 K meaning either transit in Mercury perihelion or solar probe like missions. Further, previous studies on high temperature solar arrays [43] showed that better solar cell survivability can be achieved through changes to the contact metallization and through the use of diffusion barriers in the GaAs cells. The same improvement could be applied to PETE, in order to extend the thermal stability operation of the device.

In terms of future work, we are exploring the possibility to increase the emitted current, and thus the efficiency, by nanostructuring the back surface using cone structures. Additionally, in order to reduce the effect of the electron charge cloud we are considering the insertion of an electrostatic grid (gate) between cathode and anode.

Acknowledgment

This work was supported by the European Space Agency contract No 4000112049/14/NL/MV under the GSP/ARIADNA program. JB and JML also acknowledge the financial support of MINECO (ENE2012-37804-C02-02 and AIC-B-2011-0806) and Community of Madrid (S2013/MAE-2780).