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GaAs Near-Field Thermophotonic Devices: Approaching The Idealized Case With One-Dimensional PN Junctions

Julien Legendre^{a,*}, Pierre-Olivier Chapuis^a

^aUniv Lyon, CNRS, INSA-Lyon, Université Claude Bernard Lyon 1, CETHIL UMR5008, F-69621, Villeurbanne, France

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ABSTRACT

Thermophotonics (TPX) is a technology close to thermophotovoltaics (TPV), where a heated light-emitting diode (LED) is used as the active thermal emitter of the system. It allows to tune the heat flux, by means of electroluminescence, to a spectral range matching better the gap of a photovoltaic cell. The concept is extended to near-field thermophotonics (NF-TPX), where enhanced energy conversion is due to both electric control and wave tunneling. We perform a thorough numerical analysis of a GaAs-based NF-TPX device, by coupling a near-field radiative heat transfer solver based on fluctuational electrodynamics with an algorithm based on a simplified version of the drift-diffusion equations in 1D. Through the investigation of the emission and absorption profiles in the LED and the photovoltaic (PV) cell, and the scrutiny of the impact of key parameters on the performance of the device, we highlight the necessity to model precisely the charge transport in both the LED and the PV cell for obtaining accurate results. We also demonstrate that the performance obtained with this algorithm can approach idealized cases for improved devices. For the considered simplified architecture and 300 K temperature difference, we find a power density output of $3 \text{ kW}\cdot\text{m}^{-2}$, underlining the potential for waste heat harvesting close to ambient temperature.

1. Introduction

The necessity of a change in our relation with energy needs no longer to be proven. This change has to happen on several important topics: the generation of clean energy, the reduction of consumption of machines and buildings, and the recuperation of energy losses. On this last subject, recent solid-state heat engines avoid notably (potentially polluting) refrigerants and moving parts (thus vibrations). Thanks to these benefits, solid-state heat engines can be interesting candidates for both terrestrial and spatial applications.

Several of these engines have seen good recent development in the last 20 years thanks to dynamic research [1, 2]: we can cite thermoelectric devices [3, 4], thermophotovoltaic (TPV) devices [5], thermionic devices [6, 7] or hot-carrier cells [8, 9]. In the TPV field, if a large fraction of the research focuses on the development of improved emitters [10] or rear-face reflectors [11], advanced concepts are also under development [12], including hybridization with thermionic devices [13, 14], near-field (NF) enhancement [15, 16, 17] and thermophotonics (TPX) [18, 19]. In this work, we aim to study the combination of these last two concepts through the numerical analysis of a near-field thermophotonic (NF-TPX) device [20].

In a near-field thermophotovoltaic device (NF-TPV), by decreasing the gap distance between the emitter and the photovoltaic (PV) cell to the order of hundreds of nanometers or below, evanescent waves start to participate to the heat transfer along with propagative modes [21]. Heat transferred to the PV cell can then be increased by a factor 10 to even 100 for small gap distances [15], exceeding therefore the

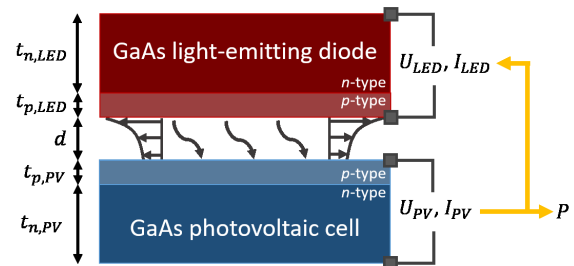


Figure 1: Schematic of a GaAs near-field thermophotonic device. The LED is maintained at 600 K, while the PV cell is kept at 300 K. In the nanogap, propagative and evanescent modes participate to the radiative heat transfer. Absorption of the radiation by the photovoltaic cell allows for the production of electrical power, a fraction of which is redirected towards the light-emitting diode for enhancement of the radiative heat transfer by electroluminescence.

blackbody limit and increasing by a similar order of magnitude the electrical power produced by the PV cell. However, the emitter cannot be controlled dynamically. The practical capabilities of such device have already been demonstrated [22, 23, 24, 25].

Thermophotonic devices rely on the recent development of light-emitting diodes (LED). Thanks to the electroluminescent effect, the emission spectrum of the LED can be tuned by the application of a voltage, and can also exceed the blackbody limit. If most of this development was directed towards lighting applications, recent research has pointed out the interest of LEDs for thermodynamic applications as an electroluminescent refrigerator/heat pump [26, 27, 28] or as a key part of a TPX device. In the latter, the LED is placed in front of a PV cell and is heated above ambient temperature

*Corresponding author

✉ julien.legendre@insa-lyon.fr (J. Legendre)
ORCID(s): 0000-0001-7316-1954 (J. Legendre)

(in a heat engine configuration). Thanks to the electroluminescence effect, the radiative power transferred to the PV cell can be increased by order of magnitudes compared to the TPV case [18]. However, the LED is consuming electrical power: a TPX device can therefore produce electrical power only when made of high-efficiency LED and PV cell, this last argument being the reason of the recent interest in the device. Indeed, with the maturation of the LED technology, the achievable efficiency has increased largely in the last decades. Among the well-known semiconductors regularly used for PV and TPV applications, gallium arsenide (GaAs) junctions has reached extremely high internal and external quantum efficiencies (above 99% [29]), making it an ideal candidate for TPX application as underlined by the Aalto group [28], even with a larger bandgap energy than what is usually used for TPV (i.e. closer to visible than to mid-infrared).

By combining near-field effects with electroluminescent enhancement in a NF-TPX device, the radiative heat transfer increase is coupled and permits a dramatic increase of the electrical power output. Due to the limited temperatures current LEDs can withstand (600 to 700 K, see the review on high-temperature pn junctions in [30]), this kind of device is ideal for low-grade heat recovery application. Note that thermoelectric devices dominate below 1000 K due to the mediocre performance of standard TPV [31]. For low temperature differences, thermodynamics limits the extraction of power density.

In the first article on NF-TPX written by Zhao *et al.* [20], a 1D near-field radiative heat transfer (NF-RHT) model was coupled with a 0D detailed balance (DB) model for the computation of the currents. We propose here to analyze the performance of a GaAs NF-TPX device, by coupling a similar NF-RHT code focusing on above-bandgap photons with an improved charge carrier behaviour model relying on the solution of the simplified drift-diffusion (SDD) equations in 1D, often used in standard PV studies [32, 33].

2. Modelling

The NF-TPX device considered is shown in Figure 1. Both the LED and the PV cell are GaAs pn junction, with p-regions at the front and n-regions at the back. The LED is heated at 600 K, which allows for large radiative heat transfer while keeping the quantum efficiency high [34, 35]. The PV cell is kept at ambient temperature (300 K). On the left of the figure is shown the geometry of the device, i.e. the thickness of the different layers and the gap distance. The main device parameters are shown in Table 1. On the right are presented the main electrical parameters, where U is the voltage and J the current density. P represents the electrical power density produced by the device.

The modelling process can be divided into two main steps:

- calculation of the near-field radiative heat transfer for above-bandgap photons (see Section 2.1)

Table 1

Device parameters. The first value given is related to the LED, the second one to the PV cell. Opt. 1 refers to the optimized values obtained with surface recombinations, Opt. 2 to those obtained without surface recombinations (see Section 4.3).

Parameter	Unit	Symbol	Ref.	Opt. 1	Opt. 2
Temperature	K	T	600 300		
P-region doping	cm^{-3}	N_a	10^{20} 10^{20}		
N-region doping	cm^{-3}	N_d	10^{18} 10^{18}		
Gap distance	nm	d	10		
P-region thickness	nm	t_p	400 400	10 10	10 10
N-region thickness	nm	t_n	10^4 10^4	509 3.21×10^3	54.9 2.87×10^3

Table 2

Modelling parameters.

Parameter	Unit	Symbol	Value	Reference
Bandgap energy	eV	E_g	1.42	[37]
Dielectric function	-	ϵ		[36]
Static rel. permittivity	-	ϵ_s	12.9	[38]
Electron rel. eff. mass	-	m_e^*	0.063	[38]
Hole rel. eff. mass	-	m_h^*	0.53	[38]
Electron mobility	$\text{cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$	μ_e		[39]
Hole mobility	$\text{cm}^2 \cdot \text{V}^{-1} \cdot \text{s}^{-1}$	μ_h		[39]
SRH recomb. coeff.	s^{-1}	A	3×10^5	[27]
Auger recomb. coeff.	$\text{cm}^6 \cdot \text{s}^{-1}$	C	10^{-30}	[27]
Surf. recomb. coeff.	$\text{m} \cdot \text{s}^{-1}$	S_n	5×10^2	[40]

- calculation of the I-V characteristic through the modelling of the charge carrier behaviour (see Section 2.2)

The different modelling parameters used in this work can be found in Table 2. Note that even if the variation of the bandgap energy with temperature is known [36], it is considered constant in this work for the sake of simplicity.

2.1. Near-field radiative heat transfer

The near-field radiative heat transfer between the LED and the PV cell is simulated using the Fluctuational Electrodynamics theory developed by Rytov [41], which allows for an accurate description of both propagative, frustrated and surface modes, the two latter being evanescent modes that are not properly described by the macroscopic framework. The random movement of charges at any point, characterized by the Fluctuation-Dissipation Theorem, can be linked to the electromagnetic wave perceived at any other point through Green tensors. Then, the radiated power is simply obtained as the mean value of the Poynting vector. By using Francoeur's formalism [42], the spectral photon flux density γ_ω , which is related to the spectral heat flux density q_ω as $q_\omega = \hbar\omega\gamma_\omega$, emitted at a layer s and received at a position z_l

in layer l can be expressed as

$$\gamma_{\omega,sl}(z_l) = (n_s^0 - n_l^0) \mathcal{T}_{sl}(z_l). \quad (1)$$

In this expression, n^0 is the modified Bose-Einstein distribution, which is tuned by means of electroluminescence through the value of the electrochemical potential μ (defined as the difference between the electron and hole quasi Fermi levels $\mu = E_{Fn} - E_{Fp}$)

$$n^0(\omega, \mu, T) = \begin{cases} \exp(\hbar\omega / (k_B T) - 1)^{-1}, & \hbar\omega < E_g \\ \exp((\hbar\omega - \mu) / (k_B T) - 1)^{-1}. & \hbar\omega \geq E_g \end{cases} \quad (2)$$

E_g is the gap energy, \hbar is the reduced Planck constant, ω the radiation frequency, k_B the Boltzmann constant and T the temperature.

In this work, we consider that the electrochemical potential μ is constant and equal to eU , a quite common approximation whose precision has been studied in [43]. By doing this approximation, we assume that the Bose-Einstein distribution is similar in all points of the LED (resp. PV cell), therefore that the net photon flux density between two points of the same device is null.

The other factor, $\mathcal{T}_{sl}(z_l)$, corresponds to the transmission coefficient between the layer s and any point of the layer l , and can be obtained from the transmission coefficient $\mathcal{T}_{sl}(z_s, z_l)$ between two points positioned respectively in layers s and l

$$\mathcal{T}_{sl}(z_l) = \int_{z_s} \mathcal{T}_{sl}(z'_s, z_l) dz'_s \quad (3a)$$

$$\mathcal{T}_{sl}(z_s, z_l) = \frac{k_v}{\pi^2} \Re \left(i \varepsilon''_{r1} \int_0^{+\infty} F_{\omega,sl}(k_\rho) k_\rho dk_\rho \right) \quad (3b)$$

$$F_{\omega,sl}(k_\rho) = \begin{bmatrix} g_{sl\rho\rho}^E(\omega, k_\rho, z_s, z_l) g_{sl\theta\rho}^{H*}(\omega, k_\rho, z_s, z_l) \\ + g_{sl\rho z}^E(\omega, k_\rho, z_s, z_l) g_{sl\theta z}^{H*}(\omega, k_\rho, z_s, z_l) \\ - g_{sl\theta\rho}^E(\omega, k_\rho, z_s, z_l) g_{sl\rho\theta}^{H*}(\omega, k_\rho, z_s, z_l) \end{bmatrix}. \quad (3c)$$

The terms g correspond to the different Weyl components of the Green tensors, k_ρ is the parallel component of the wavevector \mathbf{k} , k_v is the vacuum wavenumber corresponding to the given frequency ω and ε'' is the imaginary part of the dielectric function ε .

In this work, we assume that the LED and PV cell temperatures are kept constant; thus, below-bandgap photons do not have any impact on the electrical performance, and only above-bandgap photons are considered. In the following, the total photon flux density γ_{sl} is therefore defined as $\gamma_{sl} = \gamma_{\hbar\omega \geq E_g,sl} = \int_{E_g/\hbar}^{+\infty} \gamma_{\omega,sl} d\omega$.

2.2. Charge carrier behaviour

Once the spectral photon flux density γ_ω is obtained, the charge carrier behaviour can be modeled. In order to do so, we use two different methods:

- The detailed balance (DB) method (see Section 2.2.1) allows to easily obtain the current thanks to a balance between photons and charge carriers. This method has been used in the literature for the computation of the currents in a TPX device [18, 20, 28].
- The simplified drift-diffusion (SDD) method, in which the drift-diffusion equations are solved using standard approximations, is routinely used in photovoltaics [32, 33] but has not been used for TPX devices until now.

The use of these two methods allows for a complete description of the device performance. By using the DB method, we can estimate the ideal capabilities of such a system; then, thanks to the SDD method, the power output of a specific device can be obtained and its efficiency estimated in comparison to the ideal case.

2.2.1. Detailed balance (0D)

The photon flux density is known at any point of the system. In order to obtain a direct relation with the current densities, several assumptions have to be made [18]:

- absorption** - each above-bandgap photon absorbed generates a unique electron-hole (e-h) pair: $\tilde{G}_{rad} = \gamma_{abs}$ (defining $\tilde{x} = \int x dz$).
- radiative recombination** - photon recycling is neglected, thus the local radiative recombination corresponds to the photon flux density emitted towards the other device: $\tilde{R}_{rad} = \gamma_{em}$.
- non-radiative recombination** - the level of non-radiative recombinations and of thermal generation of e-h pairs is set by the Internal Quantum Efficiency (IQE): $\tilde{R}_{nonrad} = (1/\text{IQE} - 1)\gamma_{em}$ and $\tilde{G}_{nonrad} = (1/\text{IQE} - 1)\gamma_{em}(U = 0)$.

Since $J = e(\tilde{G} - \tilde{R})$, we obtain

$$\begin{aligned} J_l &= e \left[\gamma_{abs} - \gamma_{em} - \left(\frac{1}{\text{IQE}} - 1 \right) (\gamma_{em} - \gamma_{em}(U = 0)) \right] \\ &= e \left[(\gamma_{sl}(z_l^-) - \gamma_{sl}(z_l^+)) - \left(\frac{1}{\text{IQE}} - 1 \right) \right. \\ &\quad \left. (n_l^0 - n_l^0(U_l = 0)) (\mathcal{T}_{sl}(z_l^-) - \mathcal{T}_{sl}(z_l^+)) \right]. \end{aligned} \quad (4)$$

This expression can be simplified if $\text{IQE} = 1$:

$$J_l = e (\gamma_{sl}(z_l^-) - \gamma_{sl}(z_l^+)). \quad (5)$$

These two equations are developed in [18] and [28]. Note that in [20], a more thorough model has been developed. However, in the case of this work, we aim to obtain a simple and ideal (or quasi-ideal if $\text{IQE} < 1$) model, therefore refining the DB model is not of interest for us.

In the following, when using the DB method, we consider that both layers s and l are semi-infinite media, i.e. that $\mathcal{T}_{sl}(z_l^+) \approx 0$ (thus $\gamma_{sl}(z_l^+) \approx 0$). This allows to obtain ideal or quasi-ideal performances which are independent of the LED and PV cell geometries considered. In addition, when considering quasi-ideal cases, the IQE chosen is identical for the LED and the PV cell.

2.2.2. Drift-Diffusion (1D)

For a thorough modelling of a TPX system, Poisson, continuity and drift-diffusion equations should be solved simultaneously in order to obtain the local charge carriers distribution n and p , electric field inside the junction E and electron and hole currents J_n and J_p . In 1D, these equations are expressed as

$$\frac{dE}{dz}(z) = -\frac{e}{\epsilon_s} (n(z) - p(z) + N_a(z) - N_d(z)) \quad (6)$$

$$\frac{dJ_n}{dz}(z) = -e(R - G) \quad (7a)$$

$$\frac{dJ_p}{dz}(z) = e(R - G) \quad (7b)$$

$$J_n = e \cdot n(z)\mu_n E(z) + eD_n \frac{dn}{dz}(z) \quad (8a)$$

$$J_p = e \cdot p(z)\mu_p E(z) - eD_p \frac{dp}{dz}(z). \quad (8b)$$

These equations being coupled, solving the complete problem would need to implement an iterative process [40, 44]. However, standard approximations are regularly used to simplify the problem [32, 33]:

- the depletion approximation, in which the electric field is analytically defined and becomes independent of the illumination.
- the low-injection approximation, in which we assume that the illumination is low enough to have constant majority carrier densities (equal to the doping level).

By using these approximations, the problem can be decoupled, obtaining two differential equations for minority carriers to be solved in the quasi-neutral regions on the p-side and on the n-side. The doping levels selected in Table 1 have been chosen so that these approximations are valid: by taking as a reference the work from Blandre *et al.* [40], we consider that a doping level of 10^{17} cm^{-3} for both the p- and n-region would be enough to consider that the system is in the low-injection regime. In order to ensure that the approximation is correct, we use larger doping levels: a donor doping level N_d of 10^{18} cm^{-3} and an acceptor doping level N_a of 10^{20} cm^{-3} .

This differential equation is expressed for electrons in the p-region as

$$D_n \frac{d^2 \Delta n_p}{dz^2}(z_p) - \frac{\Delta n_p(z_p)}{\tau_{non-rad,n}} + G(z_p) - R_{rad}(z_p) = 0. \quad (9)$$

In this equation, Δn_p represents the variation of the electron density in the p-region compared to the equilibrium value n_{p0} . z_p corresponds to the position in the p-region, and the differential equation should be solved between the limit of the depletion region in the p-region $z_{p,dp}$ and the boundary of the region t_p . The boundary conditions are

$$\Delta n_p(z_{p,dp}) = n_{p0} \left(\exp\left(\frac{eU}{k_B T}\right) - 1 \right) \quad (10a)$$

$$D_n \frac{d \Delta n_p}{dz}(t_p) = -S_n \Delta n_p(t_p). \quad (10b)$$

Note that the differential equation and the boundary conditions are identical for holes in the n-region. S_n corresponds to the surface recombination coefficient for electrons at the front interface (see Table 2). By considering that the back electrode fully covers the rear interface, we can neglect surface recombinations for holes at this interface: $S_p = 0$. $D_{n,p}$ is the diffusion coefficient, obtained from the mobility $\mu_{n,p}$ through Einstein's equation:

$$D_{n,p} = \mu_{n,p} \cdot k_B T / e. \quad (11)$$

For the SDD method, as for the DB method, the generation of e-h pairs is computed from the results of the near-field radiative heat transfer model. In this case, however, the volumetric generation rate is needed, and can be written as

$$G_l = -\frac{d\gamma_{sl}^{abs}}{dz}(z_l) = -\frac{d(n_s^0 \mathcal{T}_{sl})}{dz}(z_l). \quad (12)$$

Similarly, we write the radiative recombination rate as

$$R_{rad} = -\frac{d\gamma_{sl}^{em}}{dz}(z_l) = -\frac{d(n_l^0 \mathcal{T}_{sl})}{dz}(z_l). \quad (13)$$

Note that in the existing literature for TPV (including in the near-field), radiative recombinations are modeled either by using a radiative recombination coefficient B [40][15] or by using an iterative process that allows for a precise modelling of photon recycling and transfer between the PV cell and the LED [43]. Of course, our modelling should tend towards precision (thus the second solution). However, in this work, we use an intermediary between these two models as shown in Eq. 13, which has several advantages:

- compared to the use of a coefficient B , using the local emission rate for computing the radiative recombinations allows to account for the influence of the geometry and of near-field effects.
- compared to the precise modelling, this method does not need any iteration, simplifying the calculations.
- the expressions of the radiative generation and recombination rates are similarly expressed for the DB and the SDD methods, allowing for an easier comparison.

The carrier lifetime related to non-radiative recombinations $\tau_{non-rad}$ is computed using classic A and C coefficients (see Table 2), taking into account Shockley-Read-Hall (SRH) recombinations and Auger recombinations:

$$\tau_{non-rad} = (A + C \cdot N^2)^{-1} \quad (14)$$

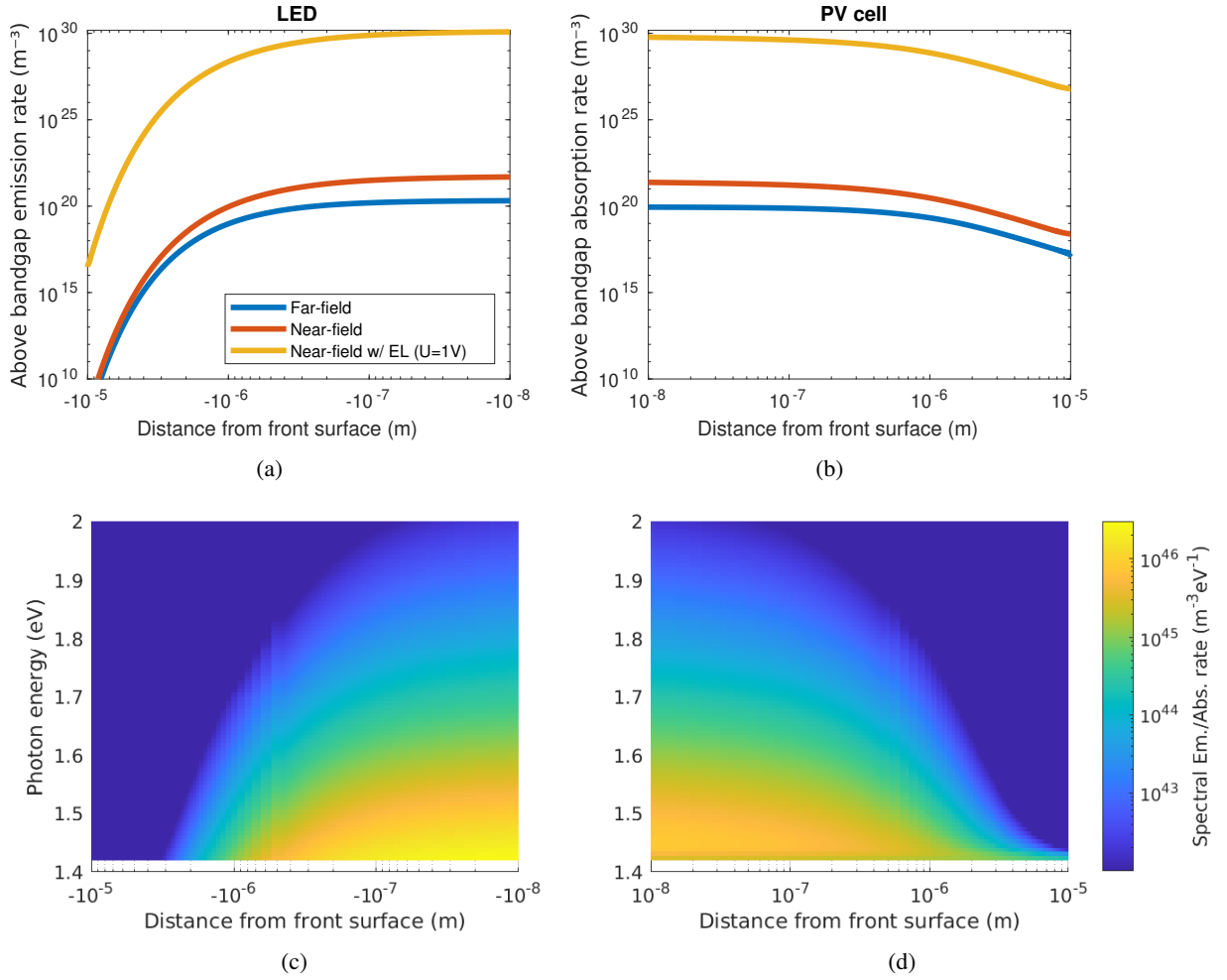


Figure 2: (a) LED emission profile and (b) PV cell absorption profile in the far-field (blue), in the near-field (orange) and in the near-field with electroluminescence, for LED and PV voltages of 1 V (yellow). The spectral profiles obtained for this last case are shown for the LED and the PV cell respectively in (c) and (d).

3. Analysis of the reference case

3.1. Absorption and Emission

Before looking at the performance of a NF-TPX device, it is interesting to study the net absorption and emission profiles at a 10 nm gap distance, respectively for the LED and the PV cell. The profiles obtained with the reference case (see Table 1) are shown in Figure 2. For the device considered, we observe as expected an extremely large increase in the absorption and emission rates, with the mean increase factor from the far-field (FF) case to the near-field (NF) case with electroluminescent enhancement reaching 10^9 . Most of this increase is due to electroluminescence: going to the near-field only accounts for a mean increase rate of the order of 10, corresponding to what was found previously in NF-TPV [15]. The dramatic effect of electroluminescence on the radiative heat transfer however comes with increased electrical power exchanged, and does not necessarily cause an increase in the electrical power density produced. This will be discussed in Section 3.3.

One can notice the similarity between the LED emission and the PV cell absorption profiles. The slight difference between these two profiles is caused by the use of a temperature-dependent dielectric function for GaAs [36]. If a temperature-independent dielectric function had been used, the profiles would have been symmetrical because of the symmetry of the device in terms of geometry and doping levels.

In Figure 2c and 2d are shown the spectral profiles. We can note the very quick decrease of the power transferred with the photon energy, with a decrease of three orders of magnitude from 1.42 eV to 1.9 eV. Therefore, only a narrow range of photon energy has an influence on the above-bandgap radiative heat transfer, thus on the device performance.

3.2. Sensitivity Study

We now investigate the global influence of two key parameters, the LED temperature and the gap distance, on the ideal performance achievable by a GaAs NF-TPX device. In order to do so, we perform a sensitivity analysis using the

DB method around the reference case (see Table 1). Results are reported in Figure 3. The LED temperature impact on the device is computed for two different IQEs of 0.9 and 1. In the ideal scenario (IQE = 1), it is shown to have only limited effect on the power output, with an increase rate of a factor 2 between 550 K and 650 K. However, this increase is much larger for lower IQE, reaching a factor 16 in the same range of temperature for IQE = 0.9. This shows the importance of using devices with nearly ideal IQE for low temperature application, as stated in the introduction.

In Figure 3b is shown the influence of the gap distance on the above-bandgap radiative heat flux and on the different electrical powers involved, for an IQE of 0.9. As shown in [45], it is interesting to study the variation of amplitude of the different modes composing the heat flux, i.e. propagative modes, frustrated modes (which propagates in GaAs but are evanescent in vacuum) and surface modes (which are evanescent on each side of the interface). Three different regions can be observed:

- above a few microns: it is the FF regime, with constant values for the different powers.
- between hundreds of nanometers and a few microns: propagative modes are still dominant in the radiative heat flux, but cavity effects cause oscillations of the powers around the far-field value.
- below hundreds of nanometers: frustrated evanescent modes become dominant, causing a large increase of the powers at first, before a slower increase below tens of nanometers. At 1 nm, surface modes are still in minority, but have exceeded propagative modes.

Looking more closely at the power levels consumed by the LED and produced by the PV cell, we can note their proximity, caused by an IQE already quite far from the ideal case and causing the net power output to be quite small compared to them. By computing the ratio between the radiative heat flux exchanged and the electrical power produced or consumed, we can obtain an estimation of the conversion efficiencies, which are

$$\eta_{PV,light-el} = \frac{P_{PV}}{q_{h\omega \geq E_g}} = 78\% \quad (15a)$$

$$\eta_{LED,el-light} = \frac{q_{h\omega \geq E_g}}{P_{LED}} = 128\%, \quad (15b)$$

showing thus the quality of the conversions. Note that the efficiency is greater than 1 for the LED because it is heated: it will still have a positive net emission even with no electrical power consumed. Since most of the power produced by the PV cell is sent back to the LED, the global conversion efficiency is much lower

$$\eta_{TPX,light-el} = \frac{P_{net}}{q_{h\omega \geq E_g}} = 2\%. \quad (16)$$

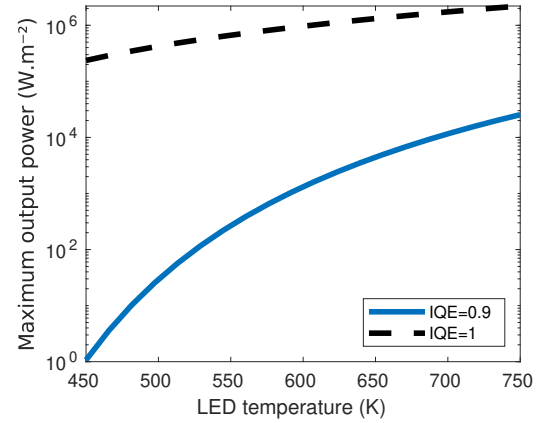
This global conversion efficiency should not be confused with the efficiency of the device, which would be expressed

as the ratio between the device power output and the heat sent to the LED in order to keep its temperature constant. We obtain

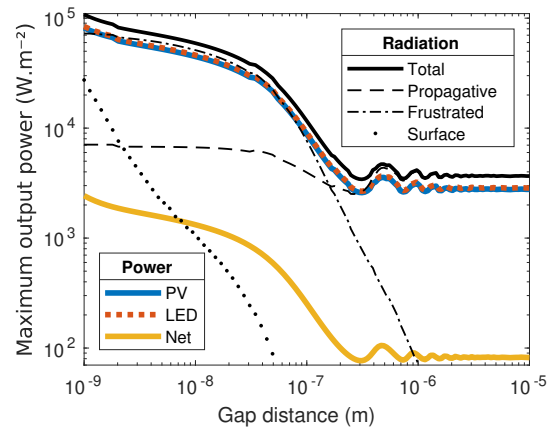
$$\eta_{TPX} = \frac{P_{net}}{q_{h\omega \geq E_g} - P_{LED}} = 9\%. \quad (17)$$

Once again, in the frame of this work, we only consider above-bandgap photons, therefore overestimating the efficiency. The scaled efficiency (i.e. the efficiency divided by the related Carnot efficiency) reaches 18%, close to what is found for NF-TPV (e.g., 23% in [15]).

We can also compute the difference between the radiative heat flux exchanged and the electrical power consumed or produced, which provides an estimate of the need for cooling the PV cell and heating the LED in order to maintain them at constant temperature. This gives around $q_{losses} = 10^4 \text{ W.m}^{-2}$ for a 10 nm gap distance (taking only into account above-bandgap photons): despite the efficient conversion, a large amount of heat will still need to be added or removed.



(a)



(b)

Figure 3: Influence of (a) the LED temperature and (b) the gap distance on the power produced by the device. For both cases, the sensitivity analysis is performed around the reference case. In (b), an IQE of 0.9 is considered.

3.3. I-V and P-V characteristics

We now take a look at the characteristics obtained for a NF-TPX device, starting with the results obtained with the DB method for an IQE of 0.9 (Figure 4a). Since both the LED and the PV cell voltages can be modulated, the characteristic of a NF-TPX device is a 3D plot. The region in which the net electrical power output is positive is strictly limited by two inequalities:

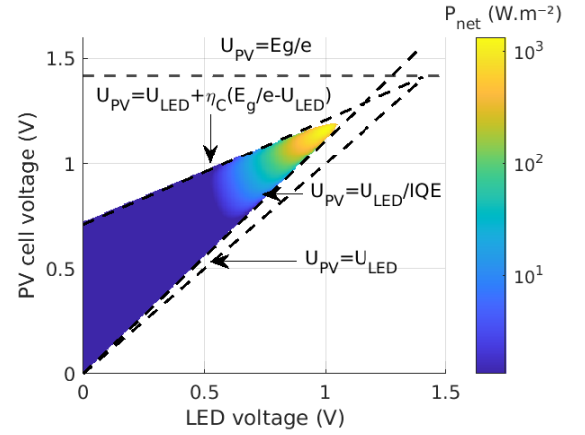
- $U_{LED} \leq U_{PV}$: with the hypothesis considered, we always have $|J_{LED}| \geq |J_{PV}|$ (they are equal if IQE = 1), having as a consequence that U_{PV} must be greater than U_{LED} in order to produce electrical power.
- $U_{PV} < E_g/e$: if the voltage reaches this value, the modified Bose-Einstein distribution diverges (in reality, this kind of voltage cannot be reached).

Even if the characteristic is limited by these two inequalities, other phenomena determine where power can be extracted from the device. For a given LED voltage, if the PV cell voltage is too large, electroluminescence from the PV cell is important enough to counterbalance the difference of temperature with the LED and change the direction of the net radiative heat flux.

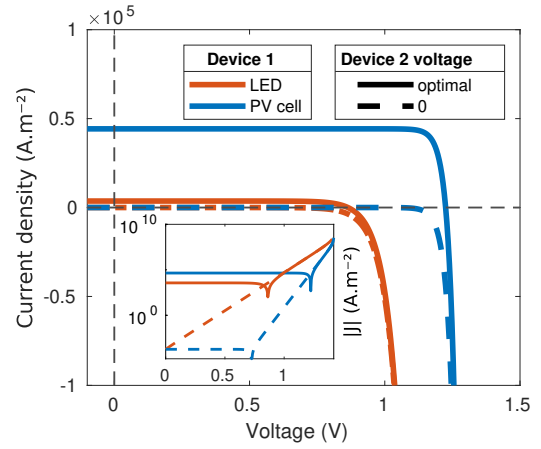
In addition, when decreasing the IQE, the range of acceptable PV cell voltage for a given LED voltage becomes narrower, resulting in the decrease of the power output. If the maximum power point (MPP) of an ideal device is close to the point $(E_g/e, E_g/e)$, the real MPP is located at lower voltages. A quick estimation of its location can be found at the intersection of two other equations that qualitatively envelop the characteristic of the device with a good precision and correspond to the two limiting factors stated above:

- $U_{PV} = U_{LED} + \eta_C (E_g/e - U_{LED})$: balance between thermally- and electrically-induced emission for the LED and the PV cell (η_C corresponds to the Carnot efficiency)
- $U_{PV} = U_{LED}/IQE$: reduction of the PV cell voltage range available with the IQE

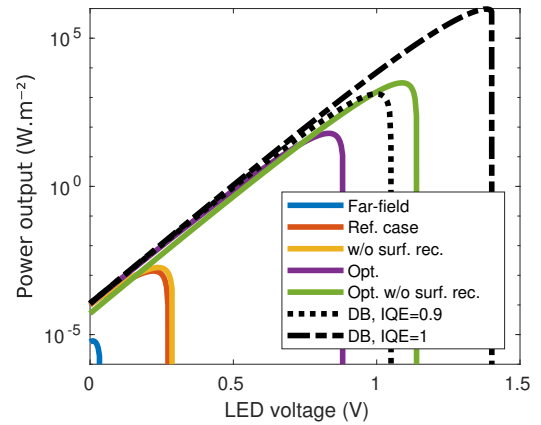
In Figure 4b, we show the I-V curve of the LED and the PV cell. The voltage given on the horizontal axis is, respectively, the LED voltage and the PV cell voltage. For the LED (resp. the PV cell) characteristic, the PV cell (resp. the LED) voltage is kept either at its optimum value (i.e. $U_{PV} = 1.16$ V and $U_{LED} = 1$ V) or at 0. For the PV cell, increasing the LED voltage (from the dashed blue line to the full blue line) raise significantly the short-circuit current by means of electroluminescence. For the LED, we can notice that the variation of the characteristic with the PV cell voltage (from the dashed orange line to the full orange line) is slower; however, for low LED voltage, electroluminescence from the PV cell is large enough to reverse the direction of the net heat flux, thus changing the sign of the short-circuit current and allowing for a power production from the LED. In this case (low LED voltage, high PV cell voltage), the LED works as a PV cell while the PV cell works as a LED. In fact, this regime where the high-temperature device is also the high-voltage device corresponds to the heat-pump/refrigerator



(a)



(b)



(c)

Figure 4: (a) Full V-V characteristic of the device, obtained with the 0D model and for an IQE of 0.9. (b) I-V characteristics of the LED and the PV cell around the maximum power point from (a). (c) Simplified P-V characteristics of the device, where the power is computed from the full characteristics as $P(U_{LED}) = \max_{U_{PV}} P(U_{LED}, U_{PV})$.

Table 3

Maximum power point reached for the different cases studied in Figure 4c.

Method	Case	P (W.m ⁻²)	U _{LED} (V)	U _{PV} (V)
SDD	Far-field	6.1×10 ⁻⁶	0.01	0.60
	Ref. case	1.4×10 ⁻³	0.22	0.75
	W/o surf. rec.	1.8×10 ⁻³	0.24	0.76
	Optimized	6.2×10 ¹	0.83	1.08
DB	Opt. w/o surf. rec.	3.1×10 ³	1.09	1.21
	IQE = 0.9	1.3×10 ³	1.00	1.16
	IQE = 1	9.6×10 ⁵	1.39	1.4

configuration of the NF-TPX device.

In order to ease the study we will prefer in the following to use simplified characteristics, as shown in Figure 4c. In this case, we plot the variation of the power output only with respect to the LED voltage. For each LED voltage, we take the maximum power output reached for the PV cell voltages considered: $P(U_{LED}) = \max_{U_{PV}} P(U_{LED}, U_{PV})$. This way of presenting the performance has several advantages:

- the comparison of the characteristic of different devices is made easier,
- the maximum power produced by the TPX device, along with the power produced by the related TPV device (at $U_{LED} = 0$), is made more readable.

The different maximum power outputs and their respective LED and PV cell voltages are summarized in Table 3. In black is traced the characteristic obtained with the DB method, for an IQE of 0.9 and 1, with respective maximum output powers of $P_{IQE=0.9} = 1.3 \times 10^3 \text{ W.m}^{-2}$ and $P_{IQE=1} = 9.6 \times 10^5 \text{ W.m}^{-2}$. Two main domains can be observed, with a fairly linear evolution first, and a sudden decrease in the electrical power output due to the exponential variations caused by the Bose-Einstein distributions. It is also interesting to note that for an IQE of 0.9, the characteristic is nearly identical to the one obtained for IQE = 1 up to a LED voltage of 0.9 V, meaning that the reduction of the power output seems to be mainly affected by the reduction of the achievable voltage range.

In color are then plotted the results obtained with the SDD method, in the FF (blue) and in the NF (orange). The maximum performance of the device is given respectively as $P_{FF} = 6.1 \times 10^{-6} \text{ W.m}^{-2}$ and $P_{NF} = 1.4 \times 10^{-3} \text{ W.m}^{-2}$. Even in the NF, the performance of the device considered is mediocre. Still, using TPX instead of TPV shows a quite noteworthy improvement ($P_{NF-TPX}/P_{NF-TPV} \approx 14$).

In the next section, we will thus focus on the understanding of the difference in the results obtained between the DB and the SDD methods, before trying to improve the device considered.

4. Towards improved devices

4.1. Surface recombinations

A first means to increase the performance of the device is to decrease surface recombinations. By nature, these are non-idealities caused by the device (i.e., not necessarily directly related to a given material) that limit the collection of charges. In Figure 4c, we show the P-V characteristic obtained when surface recombinations are removed (in yellow). If this allows for a very moderate improvement, with the maximum power output increased by 30% compared to the reference case and reaching $P_{S=0} = 1.8 \times 10^{-3} \text{ W.m}^{-2}$, reducing the surface recombinations is still important as shown in Section 4.3.

4.2. Carrier diffusion length

Two other parameters of interest could be studied in order to search for improved performance: the carriers diffusion coefficient D (Eq. 11) and the non-radiative lifetime τ (Eq. 14). Unlike surface recombinations coefficients, these two parameters are physically only related to the material and thus cannot be changed easily. However, they provide good information about the charge carrier movement capabilities inside the device, through the diffusion length $L_{diff} = \sqrt{D\tau}$. By varying L_{diff} , we modify the distance carriers will be able to travel, a process which is thus equivalent to changing the geometry for electrons and holes, but not for photons. By doing this theoretical analysis, we can easily observe how close we could approach the ideal case; this provides information about what could be obtained when optimizing the geometry. For the sake of simplicity, this study is performed separately for the LED and the PV cell, with the other device kept as a passive emitter or receiver. We choose to change the diffusion length around the value $L_{diff,0}$ obtained using the physical parameters from Table 2. Since both D and τ change when the diffusion length varies, we force them to vary at the same rate: $L_{diff} = \sqrt{(F \cdot D_0)(F \cdot \tau_0)} = F_{L_{diff}} L_{diff,0}$. The results, shown in Figure 5, reveal that the I-V characteristic of the two devices tends towards the ideal case when the diffusion lengths considered reach a hundred times the physical value. By a really rough approximation, we could state that increasing the diffusion length by a factor F is similar to decrease the geometry by the same factor. While it is probably not possible to decrease all the dimensions by a factor 100, we can however note that the dark current is already quite close to the ideal value for $F_{L_{diff}} = 10$.

4.3. Improving the geometry

We now try to optimize the geometry in order to see if we could approach the ideal case. This optimization is performed through the *fmincon* solver of MATLAB, an algorithm searching for local minima; if this solution would not be relevant for finding the optimal geometry, since the result of the process can vary with the starting point, it however returns geometries that are improved in comparison to the reference case.

We set the thickness for each region in the range [10 nm; 10 μm], while eliminating surface recombinations. The result of

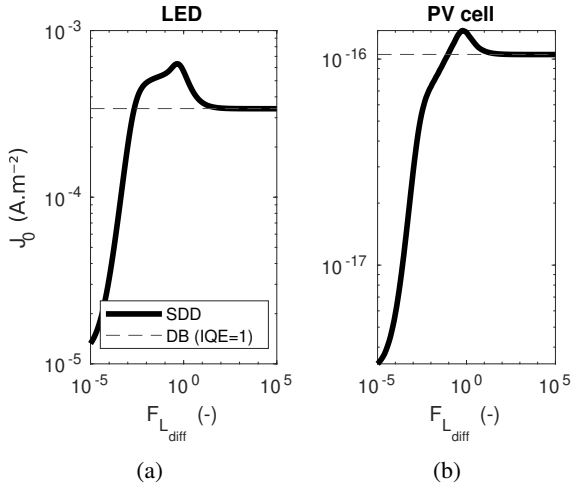


Figure 5: Impact of the diffusion length L_{diff} on the dark current of (a) an LED at 600 K, facing a GaAs absorber at 300 K and (b) a PV cell at 300 K facing a GaAs emitter at 600 K. Since the value of the diffusion length changes in the p-region and in the n-region, the variation of the dark current is shown as a function of the factor $F_{L_{diff}}$ defined as $L_{diff} = F_{L_{diff}} L_{diff,0}$. Similar tendencies are found for the short-circuit current.

this early optimization process is given in Figure 4c (green), while the improved geometry parameters are given in Table 1. The maximum power output is much larger than what was obtained for all the other cases, reaching a value of $P_{opt,S=0} = 3.1 \times 10^3 \text{ W.m}^{-2}$. It even exceeds what was obtained with the DB method for a quasi-ideal NF-TPX device with an IQE of 0.9, and reaches values obtained for FF-TPV with emitters at more than 1400 K [11]. The order of magnitude of the power output is similar to what is found for NF-TPV for 700 K temperature difference [46], and only one order below what is obtained for thermoelectric devices for 300 K temperature difference [47]. This result is essential for the development of NF-TPX device: it shows that even when getting rid of idealizing approximations, we can reach really high electrical power densities by improving both the contacts at the boundaries of the LED and the PV cell and their geometries for efficient charge carrier management. The device performance could be even further improved by optimizing the doping level of the different layers; however, the use of the SDD method limits the range of doping levels for which the result obtained is accurate. Solving instead the full Drift-Diffusion equations (see Eq. 6,7 and 8) would permit a correct optimization of the doping levels.

It is important to notice that the improvement of the geometry alone would not allow for such a large increase of the power output: when optimizing the geometry while keeping surface recombinations on the front surface (in purple in Figure 4c, see Table 1 for the geometry obtained), we reach $P_{opt} = 6.2 \times 10^1 \text{ W.m}^{-2}$. If most of the increase between the reference case (in orange) and the optimized case without surface recombinations (in green) is mainly due to the optimization of the geometry, reducing the surface

recombinations (from the purple curve to the green curve) still allows for a power increase of a factor 50.

If we analyze the geometry obtained, we can note that p-regions are only 10 nm thin (i.e., the lower bound of the thickness range tested); if reaching such thickness seems difficult to achieve, it shows nonetheless the necessity to reduce the thickness of the front layer in order to achieve high performance.

In Figure 6, we show the variation of electric field, electrostatic potential and quasi Fermi levels inside the LED and the PV cell, at the MPP. For the LED, it is clear that the depletion region extends far inside the n-region (on the left of the dashed line). In fact, at null voltage, the depletion region is at its largest and reaches the limit of the region. Since in the optimization performed, we constraint each region so that they could not be smaller than the depletion region, it means that the LED n-region thickness was also set at the minimum value possible. Thus, regarding the result of this optimization, it seems like the LED whole thickness should be set as low as possible under the mentioned approximations. We should however keep in mind that these results were obtained without surface recombinations, and for simple PN junctions; results could be quite different for complete devices.

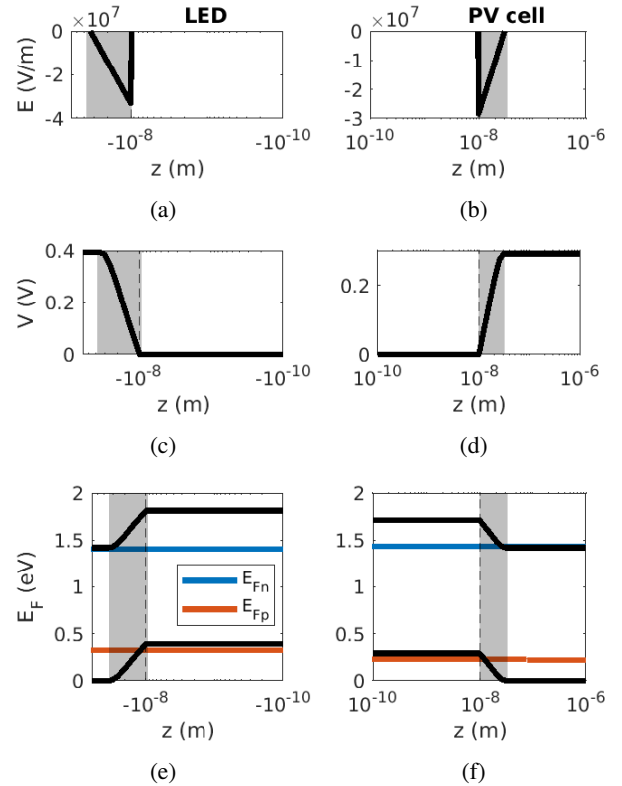


Figure 6: (a,b) Electric field, (c,d) Electrostatic potential and (e,f) Quasi-Fermi levels of the LED and the PV cell composing the device at the maximum power point reached without surface recombinations, with the optimized geometry at 10 nm. The depletion region is represented in grey.

5. Conclusion and Outlooks

We have developed a model coupling near-field radiative heat transfer and charge carrier behaviour using the Simplified Drift-Diffusion method, allowing for an accurate representation of the phenomena occurring in a near-field thermophotonic device. The difference between the results obtained with the Detailed Balance (in 0D) and the Simplified Drift-Diffusion (in 1D) shows the necessity to use the latter for a precise estimation of a device performance. By carrying an extensive analysis of a GaAs near-field thermophotonic device, we have also identified that the diffusion length and the surface recombinations have strong impacts on the performance. Through the improvement of the contacts and of the geometry, we were capable of reaching power densities as high as $P = 3.1 \times 10^3 \text{ W.m}^{-2}$, i.e. close to $10 \text{ W.m}^{-2}.\text{K}^{-1}$. This is a promising result for near-field thermophotonic devices, especially since that performance was obtained in spite of the shift of GaAs bandgap compared to the lower optimum bandgap for 600 K emitters. In addition, the doping concentrations are fixed in this study, thus not optimized.

Of course, the numerical study developed above still has room for improvement. In future work, the model itself should be improved, by getting rid of the approximation $\mu = eU$ in the modified Bose-Einstein distribution (see Eq. 2) and by solving fully the drift-diffusion equations (see Eq. 6,7,8) instead of the Simplified Drift-Diffusion. These developments have already been developed for near-field thermophotovoltaic applications respectively in [43] and [40], and could be applied to near-field thermophotonics, allowing for an accurate description of the photon recycling and of the charge carrier behaviour in general. Apart from the algorithm itself, the device considered could also be modified to approach more realistic geometries, by considering the use of pin junctions [48] and back reflectors [20].

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