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High-performance thermionic cooling devices based on tilted-barrier semiconductor heterostructures

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We study by means of full quantum simulations an asymmetric double-barrier semiconductor heterostructure refrigerator combining resonant tunneling filtering and thermionic emission. By varying the quantum well thickness, we first investigate the influence of the activation energy W on the coefficient of performance (COP) and cooling power. We show that the best performances are obtained when W equals the polar optical phonon energy of the material. However we also emphasize that cooling power and COP are severely limited by tunneling current at high bias. We then propose an original structure with a tilted potential barrier to reduce this degrading effect. Quantum simulations demonstrate that cooling properties of such tilted barrier device are significantly improved in out-of-equilibrium regime, where the thermionic cooling concept offers its best efficiency.

I. INTRODUCTION

Self-heating effect represents one of the most important technological issues in opto/nano-electronics. It results from the thermalization of hot carriers generated by high electric fields, leading to on-chip power density largely above 100 W/cm^2 and to lattice temperatures higher than four hundred kelvins^{1,2}. Such high temperatures induce significant reduction in efficiency³ and reliability⁴ of the devices. Unfortunately, thermal management is getting even more challenging in recent 3D integrated circuit architectures due to complex electrical interconnects among different device layers.

Refrigeration of electronic systems are most often based on liquid or air (fans) active cooling techniques⁵. Those approaches, which cool the entire system, cannot face the problem of temperature non-uniformity and localized hot-spots created by the nano-scaling of electronic devices. Moreover, those techniques are also extremely power consuming. For example, 40% of the energy consumed by data centers is devoted to cooling⁶. All these features make solving integrated circuit cooling one of the major scientific, technological and environmental tasks in a context of energy resource shortage^{7,8}.

Innovative cooling technologies, emerging from solid-state physics, are then urgently needed. So far, most of the studies are based on the thermoelectric Peltier effect. Thermoelectricity is a relevant solution since it is a "green" and robust method working at small scales. However thermoelectric cooling operates in the near equilibrium regime. Electrons propagate diffusively through the materials, returning part of their energy to the lattice and reducing the cooling efficiency. We then investigate nanoscaled cooling devices in which transport of electron and phonon become strongly ballistic and whose working principle applies far from equilibrium. This is the field of thermionic cooling which raises the opportunity

to obtain higher cooling efficiency than in conventional thermoelectric devices⁹.

Thermionic cooling devices have been first proposed in the 50's¹⁰ and were characterized by two metals separated by a vacuum region. The working principle was based on the fact that electrons with high thermal energy (greater than the work function of the metal) can escape from the metal. Electrons thermionically emitted from the cathode then transfer their kinetic energies to the anode to give rise to refrigeration in the cathode¹¹. However, metal-vacuum-metal based thermionic refrigerators were shown to mainly operate at high temperatures ($>700 \text{ K}$). Room-temperature refrigerators using this concept were really investigated in the 90's with the emergence of semiconductor heterostructures in which quasi-ballistic transport of electrons could occur¹²⁻¹⁴. The central vacuum region was replaced by a semiconductor heterostructure including one or several potential barriers. Lattice cooling of $\simeq 1\text{K}$ to 5K was observed at 300 K ¹⁵⁻¹⁷. However due to the strong exploratory character of the topic, the reported performances suffered from a lack of theoretical insights. The investigation of thermionic cooling devices indeed requires extensive theoretical and computational quantum modeling capable to describe electron and phonon transport at the nanometer scale. In order to capture the key aspects of the physics, we use the quantum non-equilibrium Green's function (NEGF) method. Our numerical full quantum simulations are able to take into account the thermal effects by self-consistently coupling the electron transport equations expressed within the NEGF formalism with the heat equation¹⁸.

We will focus on double-barrier asymmetric heterostructures since we recently demonstrated that such device can efficiently acts on the electronic and phononic baths refrigeration^{18,19}. We consider the device shown in Figure 1. It illustrates the band diagram of the asymmetric double-barrier heterostructure which couples "tunnel

injection” and ”thermionic extraction”. In this structure, ”cold” electrons are injected from the emitter into the GaAs quantum well (QW) via a resonant tunneling effect through a thin potential barrier (labelled as ”emitter barrier”). The role of the emitter barrier is to filter injected electrons and to concentrate the cooling in the QW. ”Hot” electrons are removed from the QW through a thermionic process above the thick AlGaAs alloy (labelled as ”collector barrier”), extracting the activation energy W from the lattice via phonon absorption. Electrons are then relaxed in the collector by emitting phonons. As a result, the QW cools and the collector heats.

In this work, we first report an extensive study of the impact of W by varying the QW thickness (L_{QW}) on the electrical and cooling properties. We demonstrate that the best cooling characteristics are obtained for W close to the polar optical phonon energy of the material, $\hbar\omega_{LO}$. Although promising, the performances are found to be degraded at high bias by the tunneling of electrons across the collector barrier. We therefore propose an original structure with a tilted potential in the collector barrier that is able to reduce this parasitic tunnel escape of electrons in the QW.

The paper is organized as follows. Section II describes the electronic quantum transport and heat transport models. In Section III we discuss the influence of the activation energy W by varying L_{QW} in terms of current characteristics, local density of states (LDOS), current spectra, and coefficient of performance (COP). From these numerical investigations, we propose an original structure with a tilted potential profile in the collector barrier and demonstrate its superiority of the cooling properties among the initial device. Finally, we draw our concluding remarks in Section IV.

II. THEORETICAL APPROACH

In order to theoretically study such a quantum device, we couple both electron and phonon transport.

A. Quantum transport for electron

Electron transport is described via the NEGF quantum formalism^{20,21}. Transport equations are expressed within the effective mass approximation to implement a one-dimensional (1D) quantum simulator along the heterostructure growth direction (x). The single band effective mass Hamiltonian describes the Γ -valley of the conduction band of the III-V semiconductors. As the considered structure is translationally invariant in the in-plane y and z directions, Born-Von-Karman periodic boundary conditions are applied on the transverse wave vector component k_t such that $k_t = n_{k_t} \times 2\pi/L_t$, with $L_t = 50$ nm and n_{k_t} an integer indexing the transverse modes whose degeneracy is equal to $\pi(2 \times n_{k_t} + 1)$ ²². In the following,

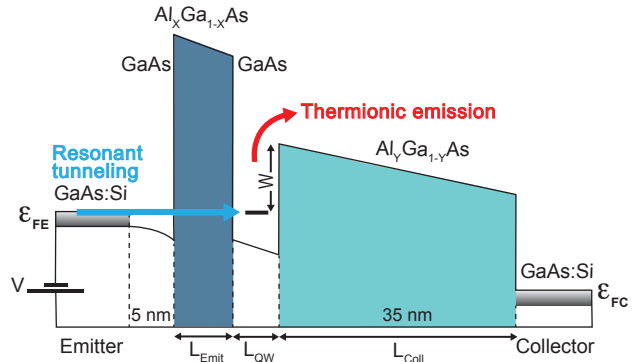


FIG. 1. (Color online) Sketch of the considered asymmetric double-barrier heterostructure. For all the considered devices, doping in the emitter and the collector is 10^{18} cm^{-3} . L_{QW} refers to the quantum well thickness and W is the activation energy, defining the gap between the QW state and the top of the collector barrier. The thicknesses of the emitter and collector barriers are $L_{\text{Emit}}=2$ nm and $L_{\text{Coll}}=35$ nm, with $X=0.4$ and $Y=0.15$ their respective aluminum concentrations, corresponding to barrier heights of 0.32 eV and 0.12 eV.

we summarize the main features of the NEGF approach in matrix notation. We first define the retarded Green’s function at the energy E for each transverse mode k_t ,

$$G_{k_t}^r = [(E - V)I - H_{k_t} - \Sigma_{L,k_t}^r - \Sigma_{R,k_t}^r - \Sigma_{S,k_t}^r]^{-1}, \quad (1)$$

where I is the identity matrix, H_{k_t} represents the effective mass Hamiltonian for the transverse mode k_t and V is the electrostatic potential energy. $\Sigma_{L/R}^r$ and Σ_S^r are the retarded self-energies for the left/right semi-infinite device contacts²³ and scattering mechanisms, respectively.

From the retarded Green’s function, the lesser/greater Green’s functions are then obtained as

$$G_{k_t}^{\lessgtr} = G_{k_t}^r \left(\Sigma_{L,k_t}^{\lessgtr} + \Sigma_{R,k_t}^{\lessgtr} + \Sigma_{S,k_t}^{\lessgtr} \right) G_{k_t}^{r\dagger}, \quad (2)$$

where the Σ^{\lessgtr} are the lesser/greater self-energies, related to their retarded counterpart by

$$\Sigma^r = \frac{1}{2} [\Sigma^> - \Sigma^<]. \quad (3)$$

Only acoustic- and polar optical-phonon interactions are considered, since non-polar-optical phonons turn out to be negligible in the semiconductors considered in this work²⁴. Interface roughness scattering is also assumed to be negligible with respect to polar optical phonon scattering. We can in particular mention the work of Lake

TABLE I. Principal NEGF parameters used in this work.

	$m_{\Gamma}^*(\text{GaAs})$	$m_{\Gamma}^*(\text{AlAs})$	$m_{\Gamma}^*(\text{Al}_x\text{Ga}_{1-x}\text{As})$	$\hbar\omega_{LO}$ (meV)	ϵ_0	ϵ_{∞}
	0.067	0.15	$x.m_{\Gamma}^*(\text{AlAs})+(1-x).m_{\Gamma}^*(\text{GaAs})$	35	12.9	10.89
Ref.	32	32	32	33	33	33

*et al.*²⁵ which clearly shows that POP scattering is significantly larger than the interface roughness contribution in GaAs/AlAs RTDs. Interaction self-energies are calculated within the self-consistent Born approximation (SCBA)^{26–28}. In our approach, the acoustic (AC) and polar optical (POP) phonon baths locally follow a Bose-Einstein distribution, and are therefore assumed at equilibrium. On the other hand, acoustic and optical phonons cannot be assumed at equilibrium with respect to each other, as the net anharmonic decay of optical phonons into acoustic plays a fundamental role in the thermal transport²⁹. This is taken into account in our model by defining, at each position of the domain, two different temperatures, T_{AC} and T_{POP} in the acoustic $\Sigma_{AC,k_t}^{\lessgtr}$ and

polar optical $\Sigma_{POP,k_t}^{\lessgtr}$ phonon self-energies respectively. As detailed in the next subsection, these temperatures are self-consistently computed by coupling the electron transport equations with the heat equation.

Interactions with both acoustic and polar optical phonons are here assumed to be local and we then consider only the diagonal part of the matrix self-energies. Such approximation has been demonstrated to be valid for acoustic phonons down to very low temperatures³⁰. To describe the POP, we adopt the diagonal expression of the scattering self-energy recently proposed as an effective description of their long-range interactions³¹. For a given wave vector k_t , it can be shown that:

$$\Sigma_{POP,k_t}^{\lessgtr}(j,j,E) = \frac{\lambda M^2}{2\pi S} \sum_{k'_t} \left[(n_L(j)+1)G_{k'_t}^{\lessgtr}(j,j,E \pm \hbar\omega_{LO}) + (n_L(j))G_{k'_t}^{\lessgtr}(j,j,E \mp \hbar\omega_{LO}) \right] \quad (4)$$

$$\times \int_{\pi/L_t}^{\pi} \frac{\pi(2n_{k'_t}+1)}{\sqrt{(k_t - k'_t \cos \theta)^2 + (k'_t \sin \theta)^2}} d\theta,$$

with $n_L(j) = (e^{(\hbar\omega_{LO})/(k_B T_{POP}(j))} - 1)^{-1}$, $M^2 = 2\pi\hbar\omega_{LO}e^2(\frac{1}{\epsilon_{\infty}} - \frac{1}{\epsilon_0})$, θ is the angle between k_t and k'_t , $S = \pi L_t^2$, and $\hbar\omega_{LO}=35$ meV. The index j indicates the x position along the discretized domain, while M is the Fröhlich factor in which ϵ_0 and ϵ_{∞} represent the static and high frequency dielectric permittivities respectively. Finally, λ is a scaling factor which takes into account for

the diagonal approximation. The value $\lambda=8$ used in this paper has been obtained within the comprehensive and physically-based analytical model proposed in Ref.31.

The total phonon scattering SCBA self-energy $\Sigma_{S,k_t}^{\lessgtr}$ for a given mode k_t can be then decomposed as :

$$\Sigma_{S,k_t}^{\lessgtr} = \Sigma_{AC,k_t}^{\lessgtr} + \Sigma_{POP,k_t}^{\lessgtr}. \quad (5)$$

Once the lesser/greater Green's function $G_{k_t}^{\lessgtr}$ of each mode k_t is determined, electron density can be calculated²⁶:

$$n_j = -2 \times \frac{i}{2\pi} \sum_{k_t} \pi(2n_{k_t}+1) \int_{-\infty}^{+\infty} G_{k_t}^<(j,j;E)dE, \quad (6)$$

$$= -i \int_{-\infty}^{+\infty} G^<(j,j;E)dE, \quad (7)$$

with $G^<(j,j;E) = \sum_{k_t} (2n_{k_t}+1)G_{k_t}^<(j,j;E)$. The carrier current density flowing from position j to $j+1$ is calculated from the off-diagonal elements $(j,j+1)$ of

$G_{k_t}^<(i,j;E)$ as

$$J_{j \rightarrow j+1} = \int_{-\infty}^{+\infty} dE \frac{e}{\hbar} \sum_{k_t} \frac{(2n_{k_t}+1)}{S} [H_{j,j+1}G_{k_t}^<(j+1,j;E) - G_{k_t}^<(j,j+1;E)H_{j+1,j}],$$

$$= \int_{-\infty}^{+\infty} \mathcal{J}_{j \rightarrow j+1}(E)dE. \quad (8)$$

where $H_{j,j+1}$ corresponds to the nearest neighbor hopping term in the discretized tight-binding like Hamiltonian and $\mathcal{J}_{j \rightarrow j+1}(E)$ is the current density spectrum (in

A/(m²·eV)). From Eq.(8) we can deduce the corresponding electronic energy current³⁴:

$$J_{j \rightarrow j+1}^E = \int_{-\infty}^{+\infty} E \mathcal{J}_{j \rightarrow j+1}(E) dE. \quad (9)$$

In practice, the set of Eqs. (1)-(5) is solved self-consistently using a recursive algorithm^{23,35} until the criteria of convergence for both electron density and carrier current density are reached. The potential energy V is self-consistently determined by nonlinearly coupling the transport equations (1)-(5) with the Poisson equation through the electron density. In all the study, band offsets are calculated based on the values reported in Ref.32. The other parameters used in the NEGF code are reported in Table I.

B. Heat transport model

Heat transport is described by solving the 1D heat equation along the x direction. The discretized heat equation on the site j reads:

$$\left[-\frac{\partial}{\partial x} [\kappa_{th}(x) \frac{\partial}{\partial x} T_{AC}(x)] \right]_j = Q_j, \quad (10)$$

where κ_{th} is the thermal conductivity. It is taken equal to the GaAs bulk value (46 W/(m·K)) in all the device, except in the QW region, where it is set to 4 W/(m·K) in order to take into account the thermal resistance associated to the interface between different layers^{36,37}. The heat equation considers the temperature of acoustic phonons, since they have a larger velocity than their polar optical counterparts and are mainly responsible of the heat transport³⁸. Left and right reservoirs are assumed to be at the thermodynamic equilibrium at $T_{AC} = 300$ K. This assumption corresponds to consider massive contacts with a sufficiently high thermal capacitance. Q_j is the volumetric source term which corresponds to the cooling power density (in W/m³) generated by electron-phonon interactions. In the framework of the previously described electron transport formalism, it can be computed as^{34,39}:

$$Q_j = -\nabla_j \cdot J^E. \quad (11)$$

A negative value of Q_j corresponds to an energy transfer from the lattice to electrons, while a positive one describes the reverse phenomenon. From a physical point of view, electrons loose or increase their energy by scattering with polar optical-phonons. In turn, optical phonons decay into acoustic phonon modes, which sustains the thermal energy propagation along the device. In stationary conditions, the power transfer from optical to acoustic phonons must be equal to the cooling power density (CPD) Q_j defined above. Within a relaxation time approximation²⁹, we can thus write

$$\frac{(T_{POP}(j) - T_{AC}(j))C_{POP}}{\tau_{POP \rightarrow AC}} = Q_j, \quad (12)$$

where $\tau_{POP \rightarrow AC}$ is the relaxation time of polar optical-phonons into acoustic phonons ($\tau_{POP \rightarrow AC} = 4.16 \times 10^{-12}$ s)⁴⁰ and C_{POP} is the thermal capacitance of the polar optical-phonons per unit volume ($C_{POP} = 1,72.10^6$ J/(m³·K))⁴⁰. The numerator of the left side expresses the average energy per unit volume exchanged between the polar optical and acoustic phonon baths in an interval $\tau_{POP \rightarrow AC}$. Eq.(12) allows us to compute $T_{POP}(j)$ from the knowledge of Q_j and $T_{AC}(j)$.

The computed values of T_{AC} and T_{POP} are substituted in Eq.(5). This establishes the coupling between the heat equation and the electron transport equations. The heat equation is iteratively solved together with the transport equations and the Poisson equation, until a global self-consistency is achieved.

III. RESULTS AND DISCUSSION

In this section we first analyze the influence of W , by varying the QW thickness, on the cooling properties. We report a comprehensive study on the involved physical effects and show that the double-barrier structure provides its best features when W is close to the polar optical phonon frequency of the material, $\hbar\omega_{LO}$. However, even in this configuration, the device undergoes performance degradations at high bias due to tunneling current across the collector barrier. Based on this observation, we propose in a second part a structure with a tilted collector barrier, leading to a significant improvement of the cooling characteristics.

Cooling properties clearly depend on the activation energy W . In the following, we then focus on the influence of W by varying the QW thickness, L_{QW} . For instance, an increase of L_{QW} will reduce the position of the quasi-localized state in the QW and will lead to an increase of W .

Figure 2 shows the current characteristics obtained for four L_{QW} varying from 4 nm to 12 nm. We can see that the current decreases when increasing the QW thickness. More precisely, device with $L_{QW}=4$ nm provides the highest current density for the entire bias range. Increasing the QW thickness to 5 nm, 6 nm and 12 nm induces a current decrease up to 40%, 55% and 70% respectively.

To understand this dependance, figure 3 shows the LDOS (top panel) and the current spectra (bottom panel) for $L_{QW}=4$ nm, 6 nm and 12 nm at $V=0.1$ V.

For $L_{QW}=4$ nm, the quasi-localized state is quite high in the QW, leading to an activation energy W of 40 meV (Figs.3-a)). Electrons can then easily escape from the QW via phonon absorption ($\hbar\omega_{LO}=35$ meV in GaAs) and hence generate a high current density (Figs.3-d)). When

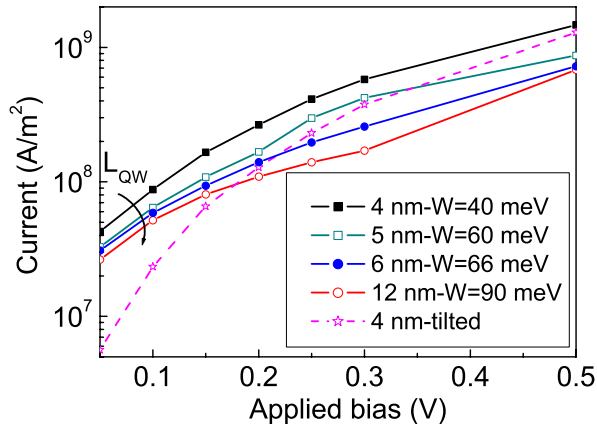


FIG. 2. (Color online) Influence of W on the current density by varying the quantum well thickness, L_{QW} , as a function of the applied bias. Four L_{QW} are considered: 4 nm (plain squares), 5 nm (empty squares), 6 nm (plain circles) and 12 nm (empty circles). The current density obtained with a tilted collector barrier is also represented for $L_{QW}=4$ nm (stars). In this latter structure, the aluminum concentration Y varies uniformly from 0.15 at the QW edge to 0.3 at the collector one, by constant steps of 5 nm.

increasing L_{QW} to 6 nm, W attains 66 meV (Fig.3-b)) which reduces significantly the thermionic current. In particular, we clearly see in Figure 3-e) two components of the current spectrum. One resulting from the resonant tunneling across the emitter barrier towards the QW state, and the second from the QW above the collector barrier. Due to the thick collector barrier, the resonant tunneling component indeed ends in the QW. For $L_{QW}=12$ nm, the first bound state continues to decrease in the well, leading to $W=90$ meV. Moreover, the second quasi-localized state now enters the QW (Fig. 3-c)), inducing a second thermionic component around 0.12 eV in the current spectrum (Fig. 3-f)). This second conducting channel is however not enough to compensate the rise of W and the total current keep decreasing.

Figure 4-a) shows the cooling power J_Q for the three previously considered L_{QW} . J_Q is obtained by integrating over x the negative part of the cooling power density Q_j (Eq.(11)). According to the definition of Q_j , a negative (positive) value of Q_j indicates a cooling (heating) of the lattice. We then only integrate the negative component of Q_j in order to get the cooling power of the entire device. Integrating also the positive component of Q_j would systematically give a final positive value equal to the applied electrical power ($P_{Elec}=J \times V$), due to energy conservation. We then remark that the entire device ("central region+contacts") always heats more than it cools but the aim is to locally efficiently cool the QW and to extract the heat as far as possible from it, in

the collector region. This is unfortunately inherent to all thermionic cooling and thermoelectric devices. The cooling power presents the same general feature for the three structures. Starting from small values at low bias, it reaches a maximum at $V=0.3$ V.

Figure 5-a) sheds light on this trend. It shows the cooling power density for $L_{QW}=4$ nm at $V=0.1$ V and $V=0.3$ V. We see that the negative component (corresponding to the cooling power) is higher at $V=0.3$ V. In particular the two dips located just before the emitter barrier and in the QW are enhanced. Those two dips correspond to phonon absorption before the emitter barrier and in the QW respectively. Indeed, as shown in the LDOS of Figure 5-b), the energy interval between the bottom of the conduction band in the emitter and the QW state is equal to W ($\simeq 40$ meV). This value is also very close to the polar optical phonon energy in GaAs ($\hbar\omega_{LO}=35$ meV). Electron in the emitter region can then be transmitted across the device by absorbing sequentially two polar optical phonons. This is also why device with $L_{QW}=4$ nm gives the highest cooling power. For higher W , several phonons are required to extract the electrons from the QW, reducing the current and therefore the power. At larger bias, the QW state first aligns and then goes below the bottom of the conduction band in the emitter. In that regime, electrons need to emit phonons before reaching the QW states. The current keep increasing, but phonon absorption and J_Q are drastically reduced. The case of $L_{QW}=12$ nm is slightly different since the cooling power is not reduced at $V=0.5$ V. This is due to the presence of the second bound state through which transport can occur and which goes below the bottom of the conduction band at higher bias. We do not discuss in more detail this phenomenon since it does influence significantly the refrigeration properties.

Figure 4-b) shows the related COP, defined as the ratio of J_Q by the applied power ($P_{Elec}=J \times V$). For all the structures the COP decreases with the bias. This feature can be simply explained by assuming that cooling power is proportional to $W \times J$. This rough approximation is valid in the case where most of the electrons are extracted at the top of the collector barrier. Distribution of electrons in the QW following the Maxwell-Boltzmann statistics, contribution of states above W decreases exponentially, and should be rather small. We indeed demonstrated both experimentally and theoretically in Ref.19 that electron extraction from the QW mainly occurs at the top of the collector barrier, leading to an evaporative cooling effect. When applying a bias, hot electrons are extracted from the QW and the remaining ones rethermalize at a lower temperature. Such effect results from the modification of the electron momentum in the QW due to elastic interactions with acoustic phonons. All these lead us to think that an electron in the QW absorbs, on average, an energy equal to W . The COP can be then written as $J_Q/P_{Elec}=(W \times J)/(V \times J)=W/V$, which appears to be inversely proportional to V . At a given bias, the COP should also be the weakest for de-

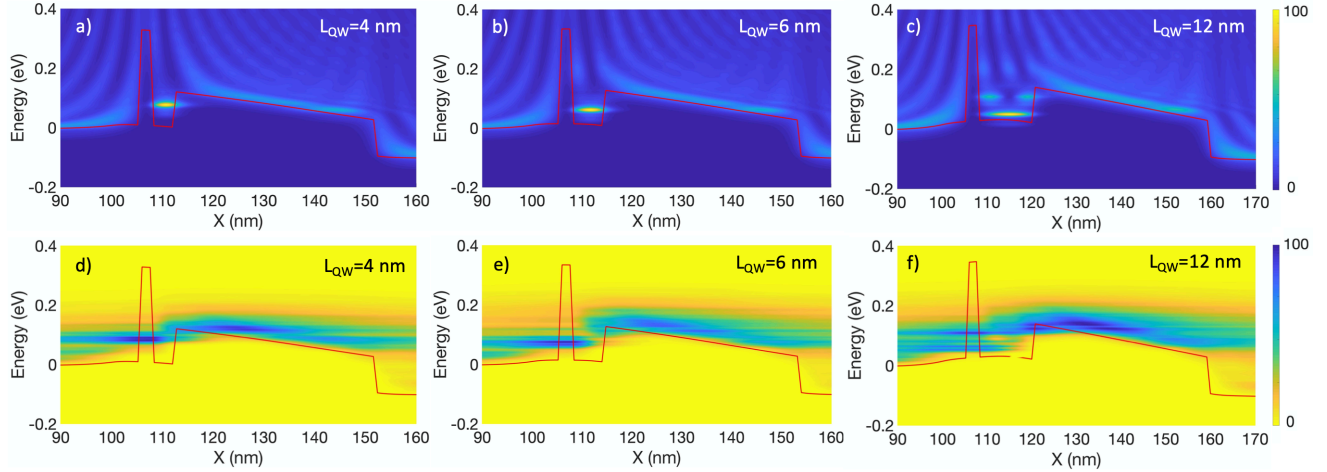


FIG. 3. (Color online) Top panel: LDOS for a) $L_{QW}=4$ nm; b) $L_{QW}=6$ nm; c) $L_{QW}=12$ nm, calculated for $V = 0.1$ V. Bottom panel: d), e), and f) are current spectra corresponding to a), b), and c). Solid red lines indicate the potential profile along the devices. The origin of the energy scale is the Fermi level of the emitter, ε_{FE} .

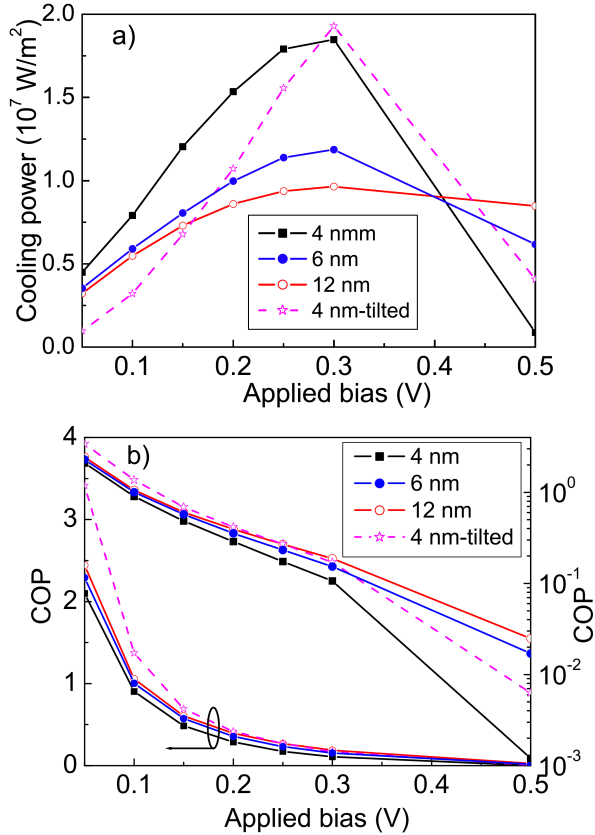


FIG. 4. (Color online) a) Cooling power (J_Q) and b) COP for three L_{QW} : 4 nm (plain squares), 6 nm (plain circles) and 12 nm (empty circles). Parameters of the tilted structure with $L_{QW}=4$ nm are also shown. In the tilted device, the collector barrier has an aluminum concentration varying from 0.15 at the QW edge to 0.3 at the collector one, by constant steps of 5 nm.

vices with the smallest W . This is indeed the case since devices with $L_{QW}=4$ nm and $L_{QW}=12$ nm report the worse and the best COP respectively.

In terms of performances, COP goes from less than one percent at $V=0.5$ V up to 250 % at $V_{RL}=0.05$ V!!! Such high COP values for low bias is physically sound as long as the integration of the cooling power density over the whole device remains equal to P_{Elec} . It also emphasizes the general dilemma of the cooling devices. Having a high COP but almost no power at low bias or having a high power but a low COP at high bias. This tendency is still valid for the different L_{QW} . We can see that the thickness providing the highest cooling power (i.e. $L_{QW}=4$ nm) presents the lowest COP. The opposite is also true.

We can finally note that COP does not decrease linearly with the applied voltage, as predicted by the simple model. Indeed, the triangular shape of the collector barrier in the high voltage regime induces a tunneling effect which deviates the actual COP from this simple model. As shown in Figure 6-a), tunneling component, indicated by the red arrow, reduces the effective W and accelerates the degradation of the COP. In order to attenuate this degrading effect, we then propose an original structure with a tilted collector barrier.

To weaken this effect, we progressively increase the aluminum concentration in the collector barrier such that the potential in this region becomes positively tilted at equilibrium, generating an additional barrier. We then take a device with $L_{QW}=4$ nm in which the collector barrier has an aluminum concentration varying from 0.15 at the QW edge to 0.3 at the collector one, by constant steps of 5 nm. The obtained cooling power and COP are also shown in Figure 4-a) and -b) respectively to be compared with the previous structures. We can see that the tilted device provides a better COP over the entire bias range (by at least 60 %) with respect to the conventional

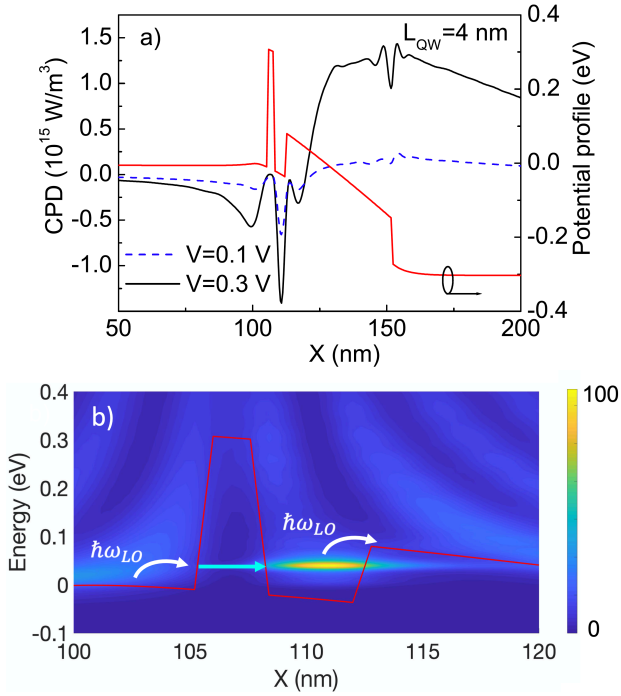


FIG. 5. (Color online) a) Cooling power density (CPD) for $V=0.1 \text{ V}$ (dashed line) and $V=0.3 \text{ V}$ (solid line); b) LDOS in the QW region at $V=0.3 \text{ V}$. On both figures, the solid red line represents the energy potential profile. $L_{\text{QW}}=4 \text{ nm}$.

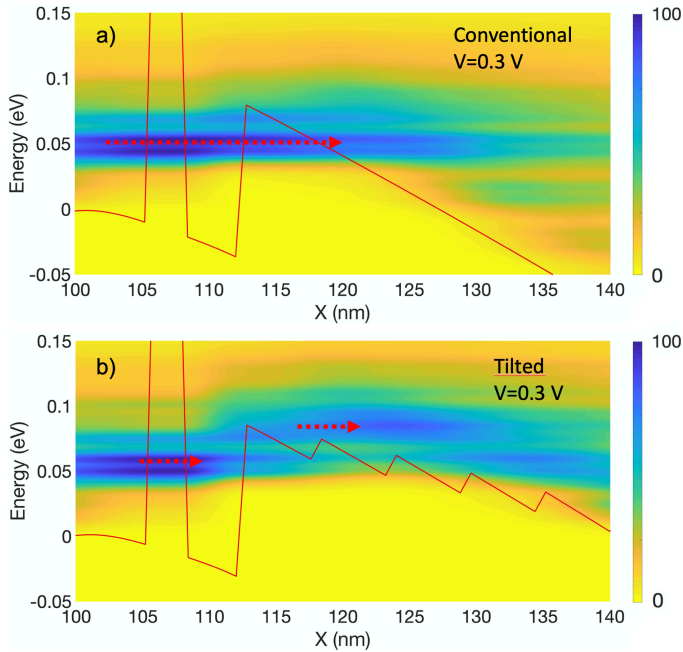


FIG. 6. (Color online) Current spectra for a) the conventional structure with $Y=0.15$ and b) the tilted one with Y varying from 0.15 to 0.3 by steps of 5 nm. The solid red lines represent the energy potential profile while red arrows indicate the electron flux through and above the collector barrier. $L_{\text{QW}}=4 \text{ nm}$ and the applied bias is $V=0.3 \text{ V}$.

structure with the same L_{QW} . Indeed the tilted collector barrier reduces the tunneling effect and increases the quantity of energy extracted by each electron, leading to a better efficiency. On the other hand, the comparison of the cooling power has two regimes. At low bias (*i.e.* $V < 0.3 \text{ V}$) the conventional device has a better performance while the tilted structure is superior at higher voltage. This behavior is explained by the current characteristics of the tilted structure also shown in Figure 2. Due to the additional potential height in the collector barrier, the tilted device presents a much weaker current. This reduction is more important at low bias when the additional barrier is larger. When increasing the bias, the tilted collector barrier is progressively removed and the current densities of the two structures are getting closer. The applied bias $V=0.3 \text{ V}$ corresponds to the tipping point where the cooling power becomes equal to the conventional structure one. We can also see by comparing Figures 6-a) and b) that the tunneling component of the current spectrum is less dominant in the tilted structure. The red arrows in Figure 6-b) show that the tilted potential allows to shift up the current spectrum above the collector barrier. We should finally note that the weak current density provided by the tilted device is another great advantage since it allows to reach highest cooling power and COP with a much lower power consumption ($P_{\text{Elec}}=J \times V$).

To summarize, at high bias, *i.e.* when the thermionic cooling structures are the most relevant, the tilted device provides similar cooling power (even a bit higher) while improving the COP by at least 60% with respect to the one of the conventional structure. Moreover, the smaller current density of the tilted device is another advantage in terms of power consumption. We should mention that properties of the tilted device strongly depend on the profile of the collector barrier. As such, the choice of the III-V compound is crucial to determine the operational efficiency. In the present work, AlGaAs is considered as a proof of concept, since the growth of this material is technologically very well established. However, the aluminum content should be less than 0.35 in order to avoid the electron scattering between the Γ - and the X -valleys, and then maintain a good electronic transport. This hinders a comprehensive assessment of the performances of a fully optimized structure. One could have a better clue of the expected final specifications, by considering other III-V compounds, like InAs/AlSb, whose conduction band offsets can be much larger than those of AlGaAs, while keeping excellent transport properties. This is however outside the scope of the present work.

Finally, let's give more general indications to improve the refrigeration properties of the device for future developments. As discussed previously, the QW is cooled, but the collector region heats. There is therefore a risk of heat backflow towards the QW. One solution to handle this detrimental effect is to consider a material in the collector barrier with a very weak electron-phonon coupling and a low thermal conductivity. We could also consider

in this region a superlattice structure since it is known that thermal conductivity of semiconductor superlattices is strongly reduced (due to interface scattering) with respect to the bulk values of their constituents⁴¹. On the opposite, reservoirs should have a high thermal conductivity in order to efficiently remove heat outside the device. In the QW, cooling performances could be also improved by choosing a material with a strong electron-phonon coupling to absorb the highest power from the lattice. Lastly, we can mention that the thickness of the emitter barrier, L_{Emit} , essentially controls the density of injected electrons in the QW. Therefore, the physical mechanisms and the general conclusions presented in this work would not be affected by considering different thicknesses.

IV. CONCLUSIONS

In this work, we theoretically investigated the performances of an asymmetric double-barrier thermionic cooling device. By varying L_{QW} , we first demonstrated that both COP and cooling power were highly dependent on the activation energy W . We showed that the highest

cooling power is obtained with an activation energy W close to the polar optical phonons frequency (i.e. $\simeq 35$ meV in GaAs). When W is above this value, the COP is slightly higher but the cooling power is substantially degraded. Moreover, it turned out that tunneling current across the collector barrier is very detrimental. In order to reduce this degrading effect, we proposed a structure with a tilted collector barrier by progressively increasing the aluminum concentration in this region. We have shown that such device improves the COP over the entire bias range while providing the same cooler power and requiring a much lower power consumption. Therefore, the present low-energy-injection/high-energy-extraction structure coupled with a tilted potential barrier may lead towards the conception of thermionic nanodevices of crucial technological interest providing unprecedented refrigeration properties.

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