PAPER

The optimum configuration design of a nanostructured thermoelectric device with resonance tunneling

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Abstract

A nanostructured thermoelectric device is designed by connecting a double-barrier resonant tunneling heterostructure to two electron reservoirs. Based on Landauer’s equation and Fermi–Dirac statistics, the exact solution of the heat flow is calculated. The maximum power output and efficiency are calculated through the optimizations of several key parameters. The optimum characteristic curve of the performance is obtained. The thermodynamic performance characteristics of thermoelectric device are analyzed, including output power and efficiency, and the optimal operation region of device is determined by optimize the main parameter. The results obtained show that the heterojunction may become a perfect energy filter by appropriately regulating the chemical potentials of electron reservoirs and optimally choosing the widths of barrier and quantum well and the nanostructured thermoelectric device with resonance tunneling may obtain simultaneously a large power output and a high efficiency.

1. Introduction

Nanostructured thermoelectric devices, which offer many advantages for energy conversion with high efficiency, have attracted considerable interest [1, 2]. With the tremendous advances of nanotechnology during the past years, a wide variety of thermoelectric devices have been proposed [3]. Mohanraman et al has summarized how the nanostructure in nanostructured composites, confinement effects in one-dimensional nanowires, and doping effects in conventional bulk composites play important roles in improving the figure of merit of thermoelectric devices [4]. Xiong et al proposed a nanostructured thermoelectric refrigerator, which is capable of cooling electrons to sub-Kelvin temperature and is particularly useful in cooling computer chips [5]. Wu et al studied three different interfacial issues of TE devices, and demonstrated that the related improvements will be beneficial for increasing their efficiencies [6]. Jang et al developed inexpensive and energy-saving technique for fabricating thermoelectric generator devices that can be employed for low-waste heat applications [7]. Nevertheless, many thermoelectric devices have the maximum theoretical efficiency that is much lower than the Carnot value due to the irreversible losses in electron transfers [8].

The performance of thermoelectric devices is determined by the figure of merit $ZT$, which remains low for most of the bulk devices. Although the conventional method for achieving high $ZT$ may increase the power factor or decreasing the thermal conductivity [9, 10], there are unexpected harvests of utilizing quantum effects at nanoscales. Paradigmatic examples are quantum dots [11, 12], heterojunctions [13], nanowires [14], and quantum point contacts [15], whose efficiencies are enhanced due to the discrete energy structure of resonant states. By using a quantum dot embedded into a semiconductor nanowire, Josefsson et al demonstrated that thermoelectric conversion efficiency can be close to the thermodynamic limit [16]. Yadollahi investigated the electronic and thermoelectric transport properties of the molecular bonds of two sided-closed single-walled boron nitride nanotubes and demonstrated that under inelastic conditions, the height of conductance peaks in the case of six atomic contacts is almost equivalent to that of single atomic contact [17]. A further insight into the
operation of the single quantum dot device included the Anderson impurity model and the master equation, which revealed that the efficiency is increased significantly by the cotunneling process [18]. Kuo et al. evaluated the properties of the electrical conductance, Seebeck coefficient, and power factor of quantum dot superlattice nanowire arrays by using the tight-binding Hamiltonian combined with the nonequilibrium Green’s function method [19]. Nakpathomkun et al. compared the performances of three low-dimensional thermoelectric systems, including zero-dimensional quantum dot with a Lorentzian transmission resonance, one-dimensional ballistic conductor, and two-dimensional energy barrier [20]. The partial thermal conductivity in solid materials is due to lattice vibrations, which requires to reveal more advanced heat transport formalisms by numerical simulation. Davier et al. presented a semi-analytical model to describe heat transport in heterostructures of length varying from the nano to the microscale [21]. Bescond et al. investigated the evaporative cooling process in a double-barrier semiconductor heterostructure thermionic refrigerator by solving the nonequilibrium Green’s function framework and the heat equation [22]. Xu et al. revealed that the lattice may be decreased by diffusive phonon temperature gradients [23].

In recent years, thermoelectric devices with resonant tunneling structures have been extensively studied due to their extraordinary advantages [24–29]. The resonant tunneling effect makes it possible to realize the ballistic transport of electrons [30], and consequently, the performance of a device depends on the energy spectrum of the tunnel. Yamamoto et al. studied the Fe/MgO/Fe (001) magnetic tunneling junction by means of the linear-response theory combined with the Landauer–Büttiker approach, where the interfacial resonant state causes the resonant tunneling and enhances the Seebeck coefficient [31]. A resonant tunneling state also occurs within the forbidden gap of the electron transmittance and creates a giant thermoelectric effect in p and n doped graphene superlattice heterostructures [32]. Castro et al. experimentally studied the optical and electronic transport properties of n-type AlSb/GaInAsSb double barrier quantum well resonant tunneling diodes, where a significant resonance current density is observed at room temperature [33]. The phonon scattering and the preparation of thermoelectric material strongly affect the performance of devices. However, reducing the size of the thermoelectric material can improve the performance due to the increased electronic density of states at the Fermi level in low-dimensional systems and quantum size effect [34].

The energy spectrum of the double barriers–quantum well structure depends on structure parameters [35–38]. One can optimize the performance of thermoelectric devices with double barrier quantum well by controlling the widths of barriers and well. However, by applying the Maxwell-Boltzmann approximation in the directions perpendicular to the direction of the current, most studies assumed that each electron removes an extra average kinetic energy \( k_B T \) from a reservoir, where \( k_B \) is the Boltzmann constant and \( T \) is the temperature of a reservoir [39, 40]. Under certain circumstances, this approximation may underestimate the magnitude of the heat flow. Therefore, for the purpose of revealing the limit of energy conversion, it is necessary to get a stricter analytical solution of thermodynamic quantities.

In the present study, we will evaluate the performance of the thermoelectric devices with Al\(_x\)Ga\(_{1-x}\)As/GaAs heterojunction by solving the exact solutions of heat fluxes. The rests of this paper are organized as follows: In section 2, the schematic of the thermoelectric device is illustrated. The electronic current density is derived based on Landauer’s formula. Fermi–Dirac (FD) statistics is used to get the exact analytical solutions of the heat fluxes flowing out of reservoirs. In section 3, the transmission probability, net electron current density, power output, and efficiency are evaluated. The lower and upper boundaries of the optimal values of main parameters are determined by maximizing the power output and efficiency. The main conclusions are summarized in section 4.

2. Model description

In semiconductor devices, electron transport is usually driven by the temperature and chemical potential differences. In our setup, two electronic reservoirs are connected by a double-barrier resonant tunneling heterostructure, as shown in figure 1(a), which consists of a quantum well of GaAs embedded between two Al\(_x\)Ga\(_{1-x}\)As barriers, and the contribution of electrons in the heterojunction may be ignored. The heterostructure allows the electron motion in the x direction completely separated from the y and z directions. Figure 1(b) indicates the wave vectors of electrons in the momentum space, where \( k_x, k_y, \) and \( k_z \) are the wave vectors in the x, y, and z directions. The electron distribution in a reservoir at temperature \( T \) and chemical potential \( \mu \) is described by the Fermi–Dirac (FD) distribution function

\[
f(E(k), \mu, T) = \frac{1}{1 + \exp((E(k) - \mu)/(k_B T))}^{-1},
\]

where

\[
E(k) = \hbar^2(k_x^2 + k_y^2 + k_z^2) / 2m^* \quad \text{expresses the dispersion relation [41] between the wave vector} \ k \ \text{and the kinetic energy of an electron,} \ h \ \text{is the reduced Planck constant, and} \ m^* \ \text{is the effective mass of electrons. The hot reservoir is at temperature} \ T_H \ \text{and chemical potential} \ \mu_{H}, \ \text{while the cold reservoir is characterized by temperature} \ T_C \ \text{and chemical potential} \ \mu_{C}.
\]
Here, we mainly focus on examining how the performance of a nanostructured thermoelectric device with resonance tunneling depends on the structure and parameters of the heterojunction, while it is a meaningful work in the future to further consider the influence of the phonon-phonon collision, phonon-electron collision, and different dispersions (such as Umklapp scattering, boundary scattering, and pore scattering) that may appear in the device. According to the description above, the net electronic current density $J_{\text{net}}$ is calculated by the difference between the electron current density flowing out of the hot reservoir and leaving that cold reservoir, which is given in supplement material A (available online at stacks.iop.org/PS/97/055701/mmedia), i.e.,

$$J_{\text{net}} = \frac{e}{2\hbar} \int_{0}^{\infty} \left[ n(\mu_{H}, T_{H}) - n(\mu_{C}, T_{C}) \right] \xi(E_{x}) dE_{x}$$

(1)

where $e$ is the elementary charge, $E_{x}$ is the energy in the $x$ direction, $n(\mu, T) = [\exp(k_{B}T / (\pi \hbar^{2})) - 1]^{-1}$, and $\xi(E_{x})$ is the transmission probability, whose concrete expression is given in supplement material B. According to the first law of thermodynamics, each electron leaving a hot reservoir carries away energy $E = \mu_{H}$ [42, 43], which is the difference between the total energy of the electron and the chemical potential $\mu_{H}$ of the hot reservoir. An electron from the cold reservoir travelling through the heterojunction will dump the energy that it removes from the cold reservoir plus the work done on it by the chemical potential bias into the hot reservoir, i.e., $E - \mu_{C} = eV$, where $V = (\mu_{C} - \mu_{H}) / e$ is the voltage of the device. Furthermore, in conventional thermoelectric device, the contribution of energy is $k_{B}T/2$ per degrees of freedom, which can be calculated by Maxwell-Boltzmann function

$$f(E_{x}) = \frac{1}{\sqrt{2 \pi m_{e} k_{B} T}} \exp \left(- \frac{m_{e} v_{x}^{2}}{2 k_{B} T} \right).$$

Thus, the total energy of electrons is the filtered energy in $x$-direction plus the average contribution from $y$-$z$ dimension, but in certain case, the distribution of electrons is determined by quantum statistics and Fermi–Dirac function is required to avoid deviation of results. Maxwell-Boltzmann (MB) statistics has been widely adopted in literatures to calculate the energy carried by electrons in the $y$ and $z$ directions [44]. As a result, the energy removed by each electron that leaves a hot reservoir is replaced by $E_{x} + k_{B}T_{H} - \mu_{H}$, where $k_{B}T_{H}$ is the average value of kinetic energy in the $y$ and $z$ directions based on the MB approximation [45]. The electron leaving the cold reservoir may arrive at the hot reservoir and deposits energy $E_{x} + k_{B}T_{C} - \mu_{C} + eV$. The net heat flux flowing out of the hot reservoir concerning the relevance of such approximation becomes

$$\dot{Q}_{\text{MB}}^{\text{H}} = \frac{1}{2\pi \hbar} \int_{0}^{\infty} [(E_{x} + k_{B}T_{H} - \mu_{H})n_{H} - (E_{x} + k_{B}T_{C} - \mu_{H})n_{C}] \xi(E_{x}) dE_{x}$$

(2)

A similar equation can be derived for the net heat flux $\dot{Q}_{\text{MB}}^{\text{C}}$ flowing out of the cold reservoir by using MB statistics. It is worth noting that this approximation may not be accurate under certain circumstances. This problem will be further discussed below. Thus, one has to resort to FD statistics for obtaining the optimal performance of the thermoelectric converter, and the heat flow

$$\dot{Q}_{H} = 2e \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{0}^{\infty} (E - \mu_{H}) [f(E, \mu_{H}, T_{H}) - f(E, \mu_{C}, T_{C})] \nu(k_{x}) \xi(k_{x}) \frac{dk_{x} dk_{y} dk_{z}}{2\pi 2\pi 2\pi}$$

(3)

where the factor 2 accounts for the degeneracy of electrons and $\nu(k_{x}) = \hbar k_{x} / m^{*}$ is the electron velocity in the $x$ direction, and $\xi(k_{x})$ indicates the transmission probability of an electron tunneling through the heterostructure as a function of $k_{x}$. The lengthy calculation result of $\dot{Q}_{H}$ is given by (A4) in supplement material A.
By assuming that electrons are transported through an ideal window within a narrow energy range $\delta E$, the transmission probability is given by [46]

$$
\xi(E_x) = \begin{cases} 
1 & (E_0 - \delta E/2 \leq E_x \leq E_0 + \delta E/2) \\
0 & (E_x \leq E_0 - \delta E/2; E_x \geq E_0 + \delta E/2) 
\end{cases}
$$

where $E_0$ is the central energy of the ideal window. Figure 2 shows the curves of the net heat fluxes out of the hot reservoir varying with $E_0$ based on equations (3) or A(4) in supplement material A (red dashed line) and equation (2) (black solid line), which provide a direct comparison between the exact analytical solution and the MB approximation. It is observed from figure 2 that when the window is at a range of low energy ($E_0 \lesssim 1.87$ meV), the heat flows $Q_H$ and $Q_{MB}^H$ are obviously different. The method based on the MB approximation underestimates the magnitude of the heat flow. The difference between $Q_H$ and $Q_{MB}^H$ vanishes when $E_0$ is large enough. The reason is that less electrons occupy the high energy levels in the reservoirs. Therefore, both the heat and electron flows approach zero as $E_0$ is very large. Although the MB approximation greatly reduces the complexity of calculation, the result of the heat flow may deviate from the accurate value, especially for the case that $E_0$ is not large enough. For example, at the maximum deviation position, the value calculated by the exact solution is 1.185 times that of the approximate solution. In the following discussion, the heat flow $Q_H$ will be used to evaluate the performance of the nanodevice.

3. Results and discussion

For the heterostructure shown in figure 1(a), the transfer matrix technique is used to calculate the transmission probability $\xi(E_x)$. Figure 3(a) gives the curves of the transmission probability $\xi(E_x)$ as a function of $E_x$ at $V_{bias} = 0$ V for the different widths of the barrier and well. It is clearly shown that the half peak width of the first resonance peak depends on the width $b$ of the barrier. When $w = 3.5$ nm and $b$ is changed from 3.5 nm (black dash-dotted line) to 4.0 nm (green dashed line), the first resonance peak becomes narrower as its half peak width decreases. On the other hand, the resonant energy $E_{res}$ corresponding to the maximum transmission probability $\xi_{max}$ of the first resonance peak is mainly determined by the width of the well $w$. When $b = 4.0$ nm and $w$ decreases from 3.5 nm (green dashed line) to 3.0 nm (red solid line), the first resonance peak moves to the right with higher energy level. Note that the half peak width of the first resonance peak increases slightly with the decrease of $w$ as well, as indicated by the inserted figure in figure 3(a).

In order to reveal the influences of the bias voltage, the maximum transmission probability $\xi_{max}$ of the first resonance peak and its corresponding resonant energy $E_{res}$ varying with $V_{bias}$ are presented in figure 3(b), where $b = 4.0$ nm and 3.5 nm. It is shown that $\xi_{max}$ monotonically decreases with the increase of $V_{bias}$ (black solid line), while $E_{res}$ is a monotonically increasing function of $V_{bias}$.

In the operating regime of the thermoelectric device, the thermodynamic affinity due to the temperature difference of reservoirs drives the electronic flow against the bias voltage $V_{bias}$. Figure 4 shows the electronic...
current $J_{\text{net}}$ as a function of $V_{\text{bias}}$, where the chemical potential of the cold reservoir $\mu_C = 200$ meV. The electronic flow is mainly determined by the first resonance peak, because the second resonance peak appears at the energy level much larger than $E_{\text{res}}$. Note that $E_{\text{res}}$ increases with $V_{\text{bias}}$, and less electrons exists in higher energy levels, leading to the reduction of $J_{\text{net}}$. $J_{\text{net}}$ at $b = w = 3.5$ nm (black dash-dotted line) is larger than $J_{\text{net}}$ at $b = 4.0$ nm and $w = 3.5$ nm (green solid line). This phenomenon can be explained by two aspects. The half peak width of the first resonance of $\xi(E_x)$ at $b = w = 3.5$ nm is larger than that of $\xi(E_x)$ at $b = 4.0$ nm and $w = 3.5$ nm (figure 3(a)). On the other hand, the first resonance peak moves to higher energy levels as $b$ changes from $b = 3.5$ nm to $b = 4.0$ nm, as indicated by the inserted figure in figure 4. In the case of $b = 4.0$ nm and $w = 3.0$ nm, $J_{\text{net}}$ (red solid line) is quite small compared to the other two cases in figure 4, because the transmission probability $\xi(E_x)$ shifts to energy levels with fewer electron occupation numbers. In general, both the shape and the energy range of the first resonance peak influence the electronic flow.

We consider the heat leak from the hot reservoir to the cold one by the equation of phonon radiative transfer [47].
Figure 5. The three-dimensional graphs of (a) $P$ and (b) $\eta$ varying with the chemical potential $\mu_c$ of the cold reservoir and the chemical potential difference $\Delta \mu = eV_{bias}$ where $b = 3.0$ nm, and $w = 3.5$ nm.

$$Q_L = \sigma P (T_H^4 - T_C^4)$$

where $\sigma = 1.0 \times 10^{-6}$ W cm$^{-2}$ K$^{-4}$ is the coefficient of the heat leak analogous to the Stefan–Boltzmann constant of phonon. As the temperatures of the reservoirs are below 10 K, the thermal conduction due to the electron–phonon interaction is weak and may be neglected. The power output $P$ and efficiency $\eta$ of the thermoelectric device are, respectively, expressed as

$$P = J_{net} V_{bias}$$

and

$$\eta = P / (\dot{Q}_H + \dot{Q}_L)$$

Figure 5 gives the three-dimensional graphs of $P$ and $\eta$ varying with the chemical potential $\mu_c$ of the cold reservoir and the chemical potential difference $\Delta \mu$. For a given value of $\mu_c$, $P$ first increases as $\Delta \mu$ increases. After $P$ reaches a maximum value, the electronic flow $J_{net}$ is dramatically reduced (figure 4) as $\Delta \mu$ continues to increase, resulting in the decrease of $P$. Similarly, $P$ is not a monotonic function of $\mu_c$. It is observed from figure 5(a) that when $\mu_c$ and $\Delta \mu$ are, respectively, equal to their respective optimal values $\mu_{c_0} = 206.5$ meV and $\Delta \mu_0 = 0.60$ meV, the power output attains its local maximum. Figure 5 shows that the local maximum power output and efficiency are two different states. When $\mu_c$ and $\Delta \mu$ are, respectively, equal to their respective optimal values $\mu_{c_0}$ and $\Delta \mu_0$, the efficiency attains its local maximum. Figure 5 also shows that $(\mu_{c_0}, \Delta \mu_0) > (\mu_{c_0}, \Delta \mu_0)$.

For the given values of $\mu_c$ and $\Delta \mu$, one can also plot the three-dimensional graphs of $P$ and $\eta$ varying with the barrier width $b$ and well width $w$, as indicated by figures 6(a) and (b), respectively. It is seen from figure 6 that both $P$ and $\eta$ are not monotonic functions of $b$ and $w$, and the local maximum power output and efficiency are also two different states. When $b$ and $w$ are, respectively, equal to their respective optimal values $b_0 = 2.752$ nm and $w_0 = 3.491$ nm, the power output attains its local maximum. When $b$ and $w$ are, respectively, equal to their respective optimal values $b_0$ and $w_0$, the efficiency attains its local maximum. It can be seen without difficulty that $b_0 > b_p$ and $w_0 > w_p$. The line connected by star in figure 6(a) represents the stopping energy level, where the current driven by the temperature-gradient $\Delta T$ in the forward direction is compensated accurately by the bias driven current flowing in the opposite direction. The white region in the upper left corner of figure 6(a) is not the operation regime of the heat engine, where the electron flows from the cold reservoir to the hot reservoir along the chemical potential difference $\Delta \mu$. In addition, in the working region of the heat engine, the power output increases initially and then decreases with the increase of the barrier width $b$ and well width $w$, respectively. It should be noted that the power reduces and vanishes to zero with the decrease of the well width and the increase of the barrier width (lower right part of figure 6(a)). It can be explained by the fact that the decrease of the well width and the increase of the barrier width also contribute to the resonance energy level $E_{res}$ to shift to higher energy levels (along the direction of green arrow), where less electrons can be transmitted from the occupied state of the hot reservoir to the cold reservoir. In general, the heat engine cannot work at the maximum output power and maximum efficiency simultaneously. Thus, an optimally working region is required to trade off the efficiency and power. Figure 6(b) shows that the efficiency increases to its maximum and then decreases with respect to $b$ and $w$, and the local maximum efficiency is obtained at $b_0 = 3.960$ nm, $w_0 = 3.498$ nm.
When four parameters $\mu_C$, $\Delta \mu$, $b$, and $w$ are optimized simultaneously, one can obtain the characteristic curve of the efficiency versus power output, as shown in figure 7, where $\eta_P$ is the efficiency at the maximum power output $P_{\text{max}}$ and $P_{\eta}$ is the power output at the maximum efficiency $\eta_{\text{max}}$. $P_{\text{max}}$ and $\eta_{\text{max}}$ give, respectively, the upper bounds of the power output and efficiency. For a nanostructured thermoelectric device, one always wants to obtain a high efficiency and a large power output as far as possible. Thus, according to figure 7, the optimal regions of the power output and efficiency should be

$$P_{\eta} \leq P \leq P_{\text{max}}$$  \hspace{1cm} (8)

and

$$\eta_P \leq \eta \leq \eta_{\text{max}}$$  \hspace{1cm} (9)

which correspond to the green curve with negative slope shown in figure 7.

According to equations (8) and (9), one can directly determine the optimum regions of other parameters as

$$\mu_{C,\eta} \leq \mu_c \leq \mu_{C,P}$$  \hspace{1cm} (10)

$$\Delta \mu_P \leq \Delta \mu \leq (\Delta \mu)_{\eta}$$  \hspace{1cm} (11)
where \( m_h \), \( c_P \), \( m_D \), \( h_b \), \( h_w \) are the upper bounds of optimized parameters, and \( m_h \), \( c_P \), \( m_D \), \( h_b \), \( h_w \) are the lower bounds of optimized parameters. The maximum power output and efficiency and the boundary values of optimized parameters are listed in Table 1. Equations (8)–(13) and Table 1 may provide the optimal selection criteria for the main parameters of nanostructured thermoelectric devices.

### 4. Conclusions

A one-dimensional double-barrier resonant tunneling heterojunction has been adopted to study the thermoelectric performance of a nanostructured device. When electrons are transported at low energy levels, the heat flow calculated by the MB approximation is found to be always less than that obtained from the exact analytical solution and the value calculated by the exact solution is 1.185 times that of the approximate solution at the maximum deviation position. The transfer matrix method further shows that the electron and heat flows rely on the structure parameters of the heterojunction. The power output density and efficiency have been locally maximized by optimizing the chemical potential of the cold reservoir and the bias voltage for the given barrier and well widths or optimizing the barrier and well widths for the given chemical potential of the cold reservoir and the bias voltage. The optimum characteristic curve is obtained and the maximum power output density and efficiency are calculated. The optimally working regions of the thermoelectric device are determined, and the selection criteria of main parameters are supplied. These results obtained here may promote the experiment development of the nanostructured thermoelectric devices with resonance tunneling.

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### Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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### Table 1. The optimal values of some parameters at the maximum power and efficiency. 

| Parameter | Symbol | Unit | Value 1 | Value 2 | Value 3 |
|-----------|--------|------|---------|---------|---------|
| Power output density | \( P_{\text{max}} \) | (W cm\(^{-2}\)) | 0.181 | 2.752 | 3.493 |
| Well width | \( w_P \) | (nm) | 206.8 | 206.8 | 206.8 |
| Chemical potential | \( \mu_{C,P} \) | (meV) | 0.627 | 0.627 | 0.627 |
| Efficiency | \( \eta_{\text{max}} \) | | 0.402 | 0.402 | 0.402 |
| Barrier width | \( b_P \) | (nm) | 3.836 | 3.836 | 3.836 |
| Barrier height | \( h_P \) | (nm) | 3.501 | 3.501 | 3.501 |
| Chemical potential | \( \mu_{C,h} \) | (meV) | 206.6 | 206.6 | 206.6 |
| Efficiency | \( \eta_{\text{max}} \) | (meV) | 0.705 | 0.705 | 0.705 |

\[
b_P \leq b \leq b_h
\]

\[
w_P \leq w \leq w_h
\]
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