Solid-state resonant tunneling thermoelectric refrigeration in the cylindrical double-barrier nanostructure*

Liu Nian(刘 念)[a†], Luo Xiao-Guang(罗小光)[b], and Zhang Mao-Lian(章毛连)[a]

[a] *Department of Physical and Electronics, Anhui Science and Technology University, Bengbu* 233100, *China*
[b] *Department of Physics, Southeast University, Nanjing* 211189, *China*

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A solid-state thermoelectric refrigerator with a cylindrical InP/InAs/InP double-barrier heterostructure is proposed. Based on the ballistic electron transport and the asymmetrical transmission, we derive the expressions of the performance parameters of this refrigerator. The cooling rate rather than the coefficient of performance is affected by the area of the inner cylinder. Then through the numerical simulation, a triangular cooling rate region is found with respect to the chemical potential and bias voltage; further, that it is because of the small full width at half maximum of the transmission resonance and the linear relationship between the energy position of resonance and the bias voltage. These tunable results might supply some guide to the cooling in tiny components or devices.

Keywords: thermoelectric, cooling region, double-barrier heterostructure, resonant tunneling

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1. Introduction

Thermoelectric devices have many advantages over other energy converters, including high reliability, long life, no moving parts, low maintenance requirements, low pollution, etc.[1–3] But the relatively low efficiency of the thermoelectric devices restricts their practical application. Recently, due to the development of nanotechnology, thermoelectric devices have aroused considerable interest.[4–7] By using artificially nanostructured thermoelectric materials, the efficiency of the thermoelectric device can be dramatically enhanced: it is much higher than those of their bulk counterparts. For example, Hicks and Dresselhaus proposed that the reduced dimensionality of superlattices could be used to enhance the electronic density of states and to obtain high efficiency;[8,9] Humphrey *et al.*[10] and Nakpathomkun *et al.*[11] predicted that low-dimensional super-lattices or nanowires can achieve electronic energy-conversion efficiencies approaching the Carnot limit. Beside these respects, some effective ways to increase the performance of thermoelectric devices have also been proposed.[12–16] The improvement in the efficiency of thermoelectric devices is attributed to the very low phonon heat conductivity and good electronic transport.

Most thermoelectric devices are based on the planar semiconductor nanostructure, where the interface areas of the two heat electrodes (or reservoirs) are equal. In order to improve the performance of the heterostructure cooler, Lyu and Zhang attempted to enhance the cooling efficiency in the cylindrical semiconductor nanostructure with the outer cylinder serving as the cold electrode.[17] However, their method did not contain the interaction inside the device, such as the space charge limitation.[18] Another shortcoming of their derivation is without considering the condition of electron transmission (i.e., from full to empty state) which cannot be shown directly in the planar thermoelectric devices. Following these ideas, we propose to use the cylindrical double-barrier nanostructure as the thermoelectric refrigerator in this paper, and derive the expressions of the performance parameters again. We analyze the influences of the chemical potential and the bias voltage on the performance of the thermoelectric refrigerator.

2. Cylindrical thermoelectric refrigerator mode

The schematic diagram of the cylindrical thermoelectric refrigerator with the inner cylinder serving as the cold electrode is shown in Fig. 1. R_C and R_H are the radii of the inner and outer cylinders, which can be regarded as cold and hot electrodes (parts I and II in Fig. 1) in contact with the cold and hot environment respectively. There is an InP/InAs/InP double-barrier nanostructure between the two electrodes with barrier and well widths of b and w. We assume that the cold and hot electrodes, which are also made of InAs, couple well with environments with different chemical potentials $\mu_C > \mu_H$ and different temperatures $T_C < T_H$. The barrier height is φ, and a bias voltage V_0 is applied to the two electrodes, then $\mu_C = \mu_H + |eV_0|$.

Generally and macroscopically, under the energy selection of the InP/InAs/InP double-barrier nanostructure, the electrons in the two electrodes can be mutually exchanged

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†Corresponding author. E-mail: lnlive@163.com

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by tunneling. The electrons tend to transmit from high to low chemical potentials/temperatures.[10] So the direction of the net electron current in the device can be tuned artificially. From the microcosmic view, the differences between chemical potentials and temperatures of the two electrodes cause the difference in the Fermi–Dirac distribution function $f_{\mathrm{C/H}} = 1/\left\{\exp\left[\left(E-\mu_{\mathrm{C/H}}\right)/k_{\mathrm{B}}T_{\mathrm{C/H}}\right]+1\right\}$, where k_{B} is the Boltzmann constant and $f_{\mathrm{C/H}}$ represents the average level of the occupied states of electrons. In other words, the electronic empty rate is $1-f_{\mathrm{C/H}}$. Theoretically, the transmission direction of the exchanged electrons should be from an occupied state to an empty state. That means that several conditions must be satisfied to let an electron with energy E be transmitted successfully from one electrode to the other. Firstly, the electronic occupancy rate in one electrode cannot be 0; secondly, the electronic empty rate in the target electrode cannot be 0 either; and thirdly, the electrons can be allowed to transmit through the InP/InAs/InP double-barrier nanostructure. Hence we can use the function of $f_{\mathrm{C/H}}\left(1-f_{\mathrm{H/C}}\right)\zeta\left(E\right)$ to describe the transmission behavior of one electron with energy E, from a cold/hot to hot/cold electrode, where $\zeta\left(E\right)$ is the tunneling transmission probability. Moreover, only the electrons with energy E, located in the region of $k_{\mathrm{B}}T$ around the chemical potential, can be transmitted.

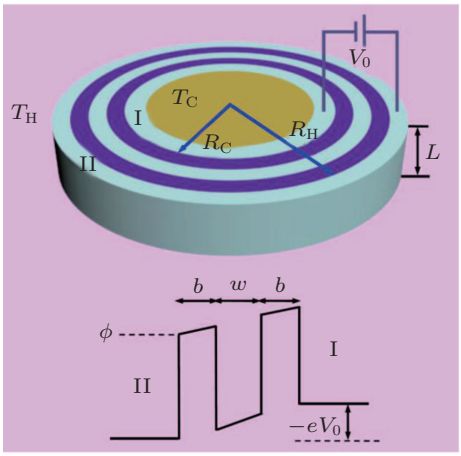


Fig. 1. (color online) Schematic diagrams of the cylindrical thermoelectric refrigerator with the inner cylinder serving as the cold electrode (upper part) and the corresponding band structure (lower part).

To analyze the performance of the cylindrical refrigerator here, two assumptions are made. One is the heat flux coupling tightly with the electron current. The cold/hot electrode will release or absorb an amount of energy $E-\mu_{\mathrm{C/H}}$ when one electron leaves from or arrives at the electrode. The other one is the states of the electrons in the electrode being proportional to the area of the electrode $A_{\mathrm{C/H}} = 2\pi R_{\mathrm{C/H}}L$, where L is the length of the cylinder. Hence the transmission will rely on the area and more electronic states (both occupied and empty ones) exist in the wider electrode. Therefore, the transmission of the electrons from the narrow to the wide electrode will be enhanced, owing to more empty states in the wide electrode. Meanwhile, it will be weakened, owing to the fact that it has fewer occupied states. By the way, the transmission of the electrons from the wide to the narrow electrode is just the reverse. It is noted that, from the Landau formula in the planar situation,[10,16] the areas have nothing to do with the transmission. So, we might suggest that the electrons in the narrow electrode can completely arrive at the wide one, but it does not work in the opposite direction. The probability related to the area of this transmission behavior, in our model, can be expressed as

$$\rho_{\mathrm{C}\to\mathrm{H}} = 1, \rho_{\mathrm{H}\to\mathrm{C}} = A_{\mathrm{C}}/A_{\mathrm{H}}. \tag{1}$$

Now, we can derive the expressions of electron current and heat flux. The electrons leaving the cold/hot electrode and arriving at the opposite one per unit time can be counted by

$$\begin{aligned} n_{\mathrm{C/H}} = {} & 2\int_{-\infty}^{+\infty}\int_{0}^{\pi}\int_{-\pi/2}^{\pi/2} A_{\mathrm{C/H}} g\left(\theta,\varphi,k_{\mathrm{r}}\right) v_p\left(\theta,\varphi,k_{\mathrm{r}}\right) \\ & \times f_{\mathrm{C/H}}\left(1-f_{\mathrm{H/C}}\right)\rho_{\mathrm{C/H}\to\mathrm{H/C}}\zeta\left(E\right)\mathrm{d}\theta\,\mathrm{d}\varphi\,\mathrm{d}k_{\mathrm{r}}, \end{aligned} \tag{2}$$

where $g\left(\theta,\varphi,k_{\mathrm{r}}\right) = \left(2\pi\right)^{-3}k_{\mathrm{r}}^2\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\varphi\,\mathrm{d}k_{\mathrm{r}}$ is the density of states (DOS) of the three-dimensional electrode, $v_{\mathrm{p}} = \hbar m^{*-1}k_{\mathrm{r}}\cos\varphi\sin\theta$ is the velocity of electrons perpendicular to the electrode surface, the factor of 2 accounts for the degeneracy due to electron spin, and m^* is the effective mass of the electron.[19] Using $E = \left(\hbar k_{\mathrm{r}}\right)^2/2m^*$ and Eq. (1), we can rewrite Eq. (2) as

$$n_{\mathrm{C/H}} = \frac{m^*A_{\mathrm{C}}}{2\pi^2\hbar^3}\int_0^{\infty} E f_{\mathrm{C/H}}\left(1-f_{\mathrm{H/C}}\right)\zeta\left(E\right)\mathrm{d}E. \tag{3}$$

Subsequently, the net electron current from the cold to hot electrode can be obtained by $n = n_{\mathrm{C}} - n_{\mathrm{H}}$. The electric current in this cylindrical thermoelectric refrigerator can be derived from $I \equiv en$, and expressed as

$$I = \frac{A_{\mathrm{C}}m^*e}{2\pi^2\hbar^3}\int_0^{\infty} E\left(f_{\mathrm{C}}-f_{\mathrm{H}}\right)\zeta\left(E\right)\mathrm{d}E, \tag{4}$$

which will be the three-dimensional Landau-like formula[16] when fixing $A_{\mathrm{C}} = A_{\mathrm{H}} = 1$ here. Equation (4) reveals that it is in vain to enhance the electric current by increasing the area of the outer electrode.

Since coupling tightly with the electron current, the heat flux without heat loss out of the cold/hot reservoir per unit time can be obtained by

$$\dot{Q}_{\mathrm{C/H}} = \pm\frac{A_{\mathrm{C}}m^*}{2\pi^2\hbar^3}\int_0^{\infty} E\left(E-\mu_{\mathrm{C/H}}\right)\left(f_{\mathrm{C}}-f_{\mathrm{H}}\right)\zeta\left(E\right)\mathrm{d}E, \tag{5}$$

from which one can see that the heat flux is also in proportion to the area of the smaller electrode. As $A_{\mathrm{C}}\to 0$, the electric current and heat flux will vanish and the thermoelectric device cannot work due to there being only one electrode existing effectively. When $\dot{Q}_{\mathrm{C}} > 0$, the device operates as a refrigerator

and $\dot{Q}_C$ is the so-called cooling rate. As a result, this asymmetric cylindrical refrigerator is equivalent to a symmetric planar structure with interface area A_C, and has a coefficient of performance (COP)

$$\varepsilon = \frac{\dot{Q}_C}{-IV_0} = \frac{\int_0^\infty E\,(E-\mu_C)\,(f_C - f_H)\,\zeta\,(E)\,\mathrm{d}E}{-eV_0\int_0^\infty E\,(f_C - f_H)\,\zeta\,(E)\,\mathrm{d}E}, \qquad (6)$$

which is unrelated to the area of the electrode, where $-IV_0$ is the power input of the refrigerator. Then, all the performance parameters such as cooling rate and COP will be obtained if the tunneling transmission probability $\zeta\,(E)$ of the electrons through the InP/InAs/InP double-barrier nanostructure is calculated.

3. Results and discussion

In the double-barrier nanostructure (InP/InAs/InP), the parameters $\varphi = 0.57$ eV, $b = w = 7$ nm, $m^*_{\mathrm{InP}} = 0.08$ m, and $m^*_{\mathrm{InAs}} = 0.023$ m are given, where m is the mass of free electrons. The transmission probability of electrons through the nanostructure can be obtained by a numerical solution from the time-independent Schrödinger equation based on the transfer matrix technique.[20] We then choose the other parameters, such as $T_H = 200$ K, $T_C = 100$ K, $R_C = 1$ μm, $L = 2$ μm for simulation. From Eqs. (5) and (6), we obtain the plots of the cooling rate and COP versus the chemical potential μ_C and bias voltage V_0 by numerical simulation as indicated by the contour plot in Fig. 2. A triangular cooling region exists in the domains of the chemical potential and bias voltage with the lower and upper edges of $\mu_C = 0.19586 - 0.5026V_0$ and $\mu_C = 0.19586 + 0.4974V_0$ respectively. Moreover, it is shown that the maximum cooling rates are close to the upper edge and the maximum COPs coincide nearly with the lower edge. With the bias voltage being big enough, the line of the maximum cooling rates will be parallel to the upper edge, as shown in Fig. 2(a). For more details, the cooling rate and COP with respect to the chemical potential μ_C are shown in Fig. 3 when $V_0 = 0.06$ V. The maximum COP is close to the Carnot value of $T_C/(T_H - T_C)$ while the cooling rate vanishes.

It is known that the electrons with the energy located in a range of $\mu_C < E < E_0$ can contribute to the cooling effect,[10,11] where $E_0 = (\mu_C T_H - \mu_H T_C)/(T_H - T_C)$ and the COP will reach the Carnot value for the electrons with $E \to E_0$. The range is only related to the μ_C and V_0 at the given parameters above; if μ_C is fixed, the quasi-cooling region of the refrigerator will be triangular in the energy and bias voltage domains as shown in Fig. 4(b). However, not all the electrons in this region are effective. The double-barrier nanostructure will filter the electrons by resonant tunneling. Using the transfer matrix technique, we obtain the transmission probabilities of the electrons with different energies, as shown in Fig. 4(a). For the electrons with energy $E < \varphi$, there is just one tunneling resonance with the full width at half maximum less than 10^{-5} eV, so that the structure will be a good filter. From the calculation, another interesting result is found that the energy values of the maximum of the resonances are linear with respect to the bias voltage, and they can be fitted well by $E = 0.195897 + 0.497403V_0$, which can be seen in Fig. 4(b).

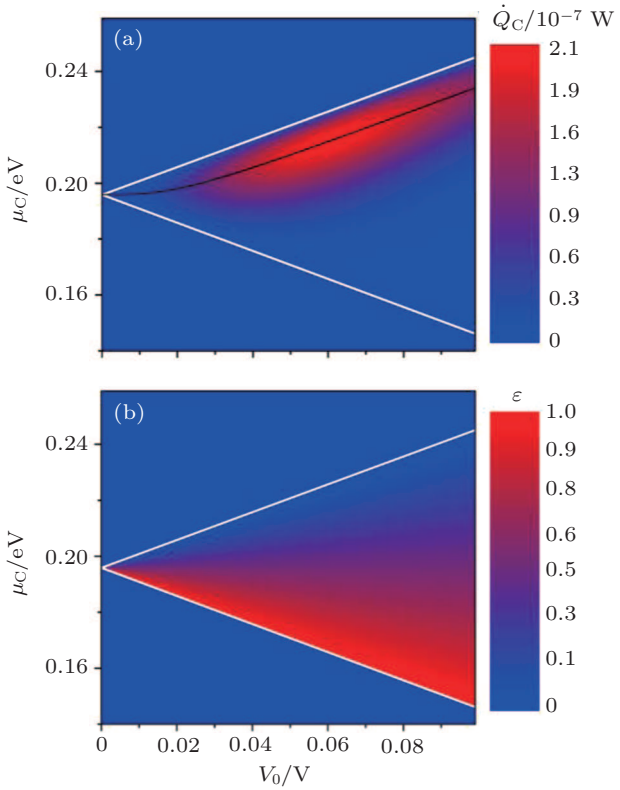


Fig. 2. (color online) Cooling rate (a) and COP (b) of the refrigerator with respect to the bias voltage and the chemical potential of the cold electrode at the given parameters. White guide lines give the cooling region and the black one denotes the maximum cooling rate.

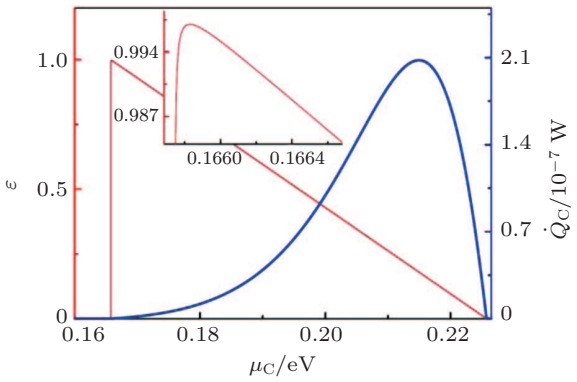


Fig. 3. (color online) Cooling rate (bold line) and COP (thin line) of the refrigerator versus chemical potential when $V_0 = 0.06$ V. Inset shows the details of the enlarged part.

Consequently, as the chemical potential μ_C increases, the electrons in the quasi-cooling region will transmit by resonant

tunneling and finally form a real cooling region, as shown in Fig. 2. The reason why the lower edge in Fig. 2 denotes the maximum COP is because the line of E_0 crosses prior to the resonance line, as seen from Fig. 4(b). The cooling region has a good triangular shape, owing to the very small full width at half maximum of the tunneling resonance.

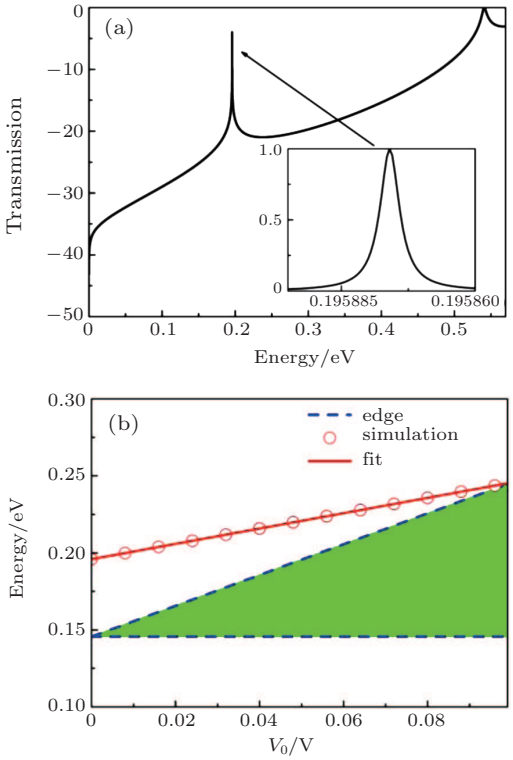


Fig. 4. (color online) (a) Transmission probability for the double-barrier structure with logarithmic vertical axis, with the inset showing the tunneling resonance. (b) The relevant position between the resonance (solid line) and the quasi-cooling region (angular area).

4. Conclusions

In this paper, we derive expressions of the performance parameters of a solid-state thermoelectric refrigerator with a cylindrical double-barrier nanostructure (InP/InAs/InP). The cooling rate rather than the COP is affected by the area of the smaller electrode, which might be used in all asymmetric thermoelectric devices. A triangular cooling region with respect to the chemical potential and bias voltage is found by numerical simulation, and it is because of the small full width at half maximum of the electron transmission resonance and the linear relationship between the position of the resonance and the bias voltage. So, the fixed or even packaged tiny thermoelectric device can work as a refrigerator by adjusting the chemical potential and bias voltage. Furthermore, it can also work as a heat engine once the tunneling resonance is located in the region of $E > E_0$, and the work region might be nearly the area (which can also be seen in Fig. 2) included between the edge of $V_0 = 0$ and the lower edge of $\mu_C = 0.19586 + 0.4974V_0$.

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