Ballistic Thermal Transistor of Dielectric Four-terminal Nanostructures

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Abstract

We report a theoretical model for a thermal transistor in dielectric four-terminal nanostructures based on mesoscopic ballistic phonon transport, in which a steady thermal flow condition of system is obtained to set up the temperature field effect of gate. In the environment, thermal flow shows the transiting behaviors at low temperatures: saturation, asymmetry, and rectification. The phenomena can be explained reasonably by the nonlinear variation of the temperature dependence of propagating phonon modes in terminals. The results suggest the possibility of the novel nano-thermal transistor fabrication.

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Rapid advances in nanometer-sized techniques have made possible the miniaturization and integration of electronic devices. Usually these device properties cannot be described by classical transport theory, since their characteristic sizes are small in comparison with the elastic mean free path between scattering events, particularly at low temperature. In this situation, the wave nature of the electrons needs to be taken explicitly into account, and electrons do not propagate diffusively instead ballistically. Based on the ballistic and phase coherent electron transport, a variety of interesting devices, e.g., the quantum stub transistor, the nanotube transistor, and the multi-terminal junctions, have been proposed.

As the counterpart of electron transport, mesoscopic phonon transport has been paid much attention recently. The new phenomenon of the universal quantum of thermal conductance at low temperature was predicted theoretically in mesoscopic dielectric systems, and verified experimentally. Some investigations of thermal transport properties have been done sequentially at the variety of nanostructures. However the thermal transistor actions in mesoscopic dielectric systems, based on quantum interference effect, have to our knowledge not been studied either theoretically or experimentally. It should have different phenomena and mechanism from that of the work based on classical theory.

In this paper, we demonstrate a theoretical model of a thermal transistor in dielectric four-terminal nanostructures (DFNSs) based on the ballistic nature of phonon transport at low temperatures, in which a steady thermal flow condition of system is obtained to set up the temperature field effect of gate. Therefore the DFNSs can work as a ballistic thermal transistor, with saturation of thermal flow from source to drain for the gate temperature at large temperature difference between the source and drain. For the asymmetric structure, thermal asymmetry and rectification are showed under changes in the temperature difference. A reasonable explanation of the phenomena is given by the nonlinear variation of the temperature dependence of propagating phonon modes in terminals. The possibility of the experimental observation of these novel phenomena is also discussed.

A two-dimensional DFNS is illustrated in Fig.1(a). Four parallel terminal wires of width \(a_i\) are directly coupled to a central ballistic window region \(V\) with width \(b\) and height \(L\) (scattering region). Other ends of four-terminal wires are connected to thermal reservoirs at equilibrium with temperatures \(T_i\), \(i = 1, 2, 3, 4\), respectively. Supposed that there is no phonon scattering inside the terminal wires and the central window, and a perfect connection between terminal wires and reservoirs, phonon scattering is solely decided by the geometrical
features and happens only at interfaces between the terminal wires and the central window.

The net thermal flow $Q_i$ in terminal wire $i$ is expressed as

$$
Q_i = \sum_{j(j\neq i)} Q_{ij} = \sum_{j(j\neq i)} \sum_{m,n} \int_{\omega_{\text{im},\text{mj}}}^{\infty} \frac{d\omega}{2\pi} \hbar \omega [n_i(\omega, T_i) - n_j(\omega, T_j)] \tilde{T}_{ji,mn}(\omega) ,
$$

(1)

where $n_i(\omega, T_i) = [\exp(\hbar \omega / k_B T_i) - 1]^{-1}$ is the Bose-Einstein distribution function of the phonons with temperature $T_i$ in the $i$-th reservoir, $k_B$ is the Boltzmann constant, and $\hbar$ is Planck’s constant. $\omega_{\text{im}} = \frac{\pi \omega_{\text{m}}}{a_i}$ is the cutoff frequency of mode $m$ in terminal wire $i$, and $v (= 5000 \text{ m} \cdot \text{sec}^{-1})$ is the group velocity. $\tilde{T}_{ji,mn}(\omega)$ is the phonon transmission coefficient that an incident phonon with energy $\hbar \omega$ from terminal $i$ at phonon mode $m$ is scattered to terminal $j$ at mode $n$, with the property: $\tilde{T}_{ji,mn}(\omega) = \tilde{T}_{ij,mn}(\omega)$. For the present DFNSs, transmission coefficient can be obtained by the mode matching method, the same approach as Ref.[6, 7]. Thermal flow $Q_{ij}$ is decided by two thermal reservoirs $i$ and $j$, and has the property: $Q_{ij} = -Q_{ji}$.

In the paper, we assume that the dielectric four-terminal system has reached the steady state. The steady thermal flow across central window from terminal 1 to terminal 4 has the definition: $Q_1 = -Q_4$, where the plus/minus sign represents separately the thermal flow into/out of system. Meanwhile temperatures of four thermal reservoirs are assumed to have the sequence: $T_1 \geq (T_2, T_3) \geq T_4$. In terms of Eq.(1) and the steady flow definition, we readily obtain the steady thermal flow condition of system:

$$
Q_{12} + Q_{13} + Q_{42} + Q_{43} = 0 .
$$

(2)

If adding the $(Q_{23} + Q_{32})$ into Eq.(2), we also get $Q_2 = -Q_3$, the steady flow between terminals 2 and 3. Obviously, the temperatures of four thermal reservoirs, which are satisfied with Eq.(2), can make the DFNS at steady state. Note that the summation of four terms in the left hand side of Eq.(2) is just the thermal flow $Q^L$ along the vertical direction of central window (region $V$), which equals zero in terms of Eq.(2), (see in Fig.1(a)). This means that the thermal flow across terminals 1 and 4 isolates from that across terminals 2 and 3 at steady state of system. With the help of Eq.(1), equation (2) transforms to

$$
[Q_{12}^*(T_1) + Q_{13}^*(T_1)] + [Q_{12}^*(T_3) + Q_{13}^*(T_3)] = [Q_{21}^*(T_2) + Q_{24}^*(T_2)] + [Q_{31}^*(T_3) + Q_{34}^*(T_3)] ,
$$

(3)

where $Q_{ij}^*(T_i)$ is the thermal flow that is produced by single thermal reservoir with temperature $T_i$ and that flows directly from terminal $i$ into terminal $j$; $Q_{ij}^*(T_i) =$
As shown in Fig.3(a), the mode spacing \( \Delta_i \) negative for a fixed gate temperature \( T \) in which the gates connect the source and drain respectively and work as controlling ends. This equation is written as

\[
\sum_m \int_{\omega_{im}}^{\infty} \frac{L}{2\pi} \hbar \omega m_i(\omega, T_i) T_{ij,m}(\omega), \quad \tilde{T}_{ij,m}(\omega) = \sum_n \theta(\omega - \omega_{jn}) \tilde{T}_{ij,mn}(\omega).
\]

In this way, the steady flow condition of system of Eq.(2) can be expressed by four single thermal reservoirs. We take reservoir 1 for the source with \( T_s = T_1 \), reservoir 4 for the drain with \( T_d = T_4 \), and reservoirs 2 and 3 for the gates with \( T_g = T_2 = T_3 \) respectively. The simplified form of Eq.(3) is written as

\[
E_1^s(T_s) + E_4^s(T_d) = E_2^s(T_g) + E_3^s(T_g), \quad (4)
\]

where \( E_1^s(T_s) = Q_{12}^s(T_s) + Q_{13}^s(T_s), E_4^s(T_d) = Q_{42}^s(T_d) + Q_{43}^s(T_d), E_2^s(T_g) = Q_{21}^s(T_g) + Q_{24}^s(T_g), \) and \( E_3^s(T_g) = Q_{31}^s(T_g) + Q_{34}^s(T_g) \). Equation (4) sets up the source-gate-drain (SGD) relation, in which the gates connect the source and drain respectively and work as controlling ends.

For a fixed gate temperature \( T_g \), a pair of corresponding temperatures \( T_s \) and \( T_d \) can be obtained from Eq.(1). Each set of temperatures including the \( T_g \) and a pair of \( T_s \) and \( T_d \) can make sure the system at steady state and be used to calculate the steady thermal flow \( Q_{sd} \) from source to drain in terms of Eq.(1); \( Q_{sd} = Q_1 \) in terminal 1 and \( Q_{sd} = -Q_4 \) in terminal 4. As stated above, we can get all values of the steady thermal flow \( Q_{sd} \) corresponding to different temperature pairs of \( T_s \) and \( T_d \) that set up the temperature difference between source and drain, \( i.e. \), \( T_{sd} = T_s - T_d \), for the fixed \( T_g \) in the DFNSs. The schematic diagrams of working procedure for \( Q_{sd} \) is shown in Fig.1(b)–(d). Furthermore, as \( Q^L = 0 \), the influence of the gate temperature \( T_g \) on the steady thermal flow \( Q_{sd} \) should be attributed to the temperature field effect (TFE). Note that all temperatures in the paper always mean those of thermal reservoirs.

For the symmetric DFNS, the inset(a) of Fig. 2 shows the calculated thermal flow \( Q_{sd} \) as a function of the temperature difference \( T_{sd} = T_s - T_d \) for five different values of \( T_g \). As seen in the figure, \( Q_{sd} \) first increases, and then tends to saturation with \( T_{sd} \) increasing for the five \( T_g \)s. In the following, we will study the phenomenon based on mesoscopic ballistic transport theory. Figure 3 illustrates the cutoff frequencies of the discrete transverse phonon modes (threshold energy) respectively in terminal 1, scattering region \( V \), and terminal 4, where the superscript \( p \) and \( n \) represent separately the positive \( T_{sd} \) at \( T_s > T_d \) and the negative \( T_{sd} \) at \( T_s < T_d \). For the symmetric DFNS with \( a_1 = a_2 = a_3 = a_4 = 20nm \), as shown in Fig.3(a), the mode spacing \( \Delta_i = \omega_{i(m+1)} - \omega_{im} = \frac{\pi}{a_i} \) in terminal 1 equals that of terminal 4. At initial state with \( T_s^p = T_d^p = T_g \), the system is at equilibrium \( (T_{sd}^p = 0, Q_{sd} = 0) \). Then the enhace of \( T_s^p \) relative to the fixed \( T_g \) excites the additional
phonon modes $\Delta m_1^p$ in terminal 1 and makes energy into terminals 2 and 3 from all modes $(m_1^{eq} + \Delta m_1^p)$ in terminal 1, in terms of $\frac{\pi \nu \Delta m_1^p}{a_1} \sim k_B |T_1^p - T_g|/\hbar$, where the superscript $eq$ represents the equilibrium state. Since $Q_1^p(T_1)$ in Eq. (3) is monotonously increasing function of temperature $T_1$, $E_1^p(T_1)$ in Eq. (3) increases correspondingly. Meanwhile, to balance the both sides in Eq. (4), $E_3^p(T_2)$ must have equal amount decreased because $E_3^p(T_2)$ and $E_3^s(T_2)$ in Eq. (4) keep constant. This means that the modes $m_4^{eq}$ in terminal 4 have $\Delta m_4^p$ decrease and the corresponding temperature $T_3^p$ drops below $T_g$ as shown in Fig.3(a). Since $\Delta m_4^p$ excited by $T_3^p$ at $T_3^p > T_g$ are higher energy modes, the decreased energy of $\Delta m_4^p$ which equals $\Delta m_4^p$ is not sufficient to cancel out the additional energy produced by $T_3^p$. Therefore $\Delta m_4^p$ in terminal 4 must be more than $\Delta m_1^p$ in terminal 1, i.e., $\Delta m_4^p > \Delta m_1^p$, in order to make the increased energy from $(m_1^{eq} + \Delta m_1^p)$ in terminal 1 and the decreased energy from $\Delta m_4^p$ in terminal 4 equal. This means that there is an unequal amount change of $\Delta m_1^p$ and $\Delta m_4^p$ for the equal amount of $E_1^p(T_1)$ increase and $E_4^p(T_4)$ decrease in Eq. (4). With $T_{sd}^p$ increasing further, as $\Delta m_1^p \sim |T_1^p - T_g|$, the ratio of $\Delta m_1^p$ to $\Delta m_4^p$ is the nonlinear monotonously decreasing; therefore $T_1^p$ shows the nonlinear increasing behavior, meanwhile $T_3^p$ has the nonlinear decreasing behavior as shown in Fig.4(a), in order to keep the system at steady state. Obviously the modes $(\Delta m_1^p + \Delta m_4^p)$ corresponding to $(T_1^p - T_3^p)$ become more with $T_{sd}^p$ increasing, but the ratio of $\Delta m_1^p$ to $(\Delta m_1^p + \Delta m_4^p)$ goes down. This means that $T_1^p$ has less contribution than $T_3^p$ for $T_{sd}^p$ increasing in terms of $\Delta m_1^p \sim |T_1^p - T_g|$. On the other hand, as the propagating channel between the source and drain consists of the propagating phonon modes $(m_1^{eq} + \Delta m_1^p)$ in terminal 1 and $(m_4^{eq} - \Delta m_4^p)$ in terminal 4, $Q_{sd}$ increases with $T_{sd}^p$; but the increment rate of thermal conductance $Q_{sd}/T_{sd}^p$ reduces with $T_{sd}^p$ increasing, i.e., $Q_{sd}/T_{sd}^p > 0$ and $\frac{d}{dT_{sd}^p}(Q_{sd}/T_{sd}^p) < 0$, (see in Fig.4(b)). Consequently, under the influence of $T_g$, the nonlinear variation of the modes $\Delta m_1^p$ and $\Delta m_4^p$ in the modes $(\Delta m_1^p + \Delta m_4^p)$ that corresponds to $T_{sd}^p$ leads to the saturation behavior of thermal flow $Q_{sd}$ in the DFNS. Furthermore, as the mode spacings in terminals 1 and 4 are identical in this symmetric structure, $Q_{sd}$ presents symmetry in the reversal of $T_{sd}^p$, i.e., $T_{d}^n > T_{s}^n$. Additionally, $Q_2 (= -Q_3)$ is two orders of magnitude lower than $Q_{sd}$.

In order to investigate the asymmetric effect, we change the DFNS from the symmetric structure to the asymmetric with $a_1 = a_2 = a_3 = 20nm, a_4 = 40nm$. As shown in Fig.2, there is asymmetry in the $Q_{sd} - T_{sd}$ behavior with thermal flow saturation for the positive and negative $T_{sd}$ for four values of $T_g$. (i) Thermal saturation discussion: for the asymmetric
DFNS, the mode spacing $\Delta_1 = \frac{\pi v}{a_1}$ in terminal 1 is twice $\Delta_4$ in terminal 4; there is a higher density of transverse phonon modes in terminal 4 as shown in Fig.3(b). When $T^p_d$ increases over $T_g$, thermal energy input from the modes $(m^{eq}_1 + \Delta m^p_1)$ in terminal 1 is canceled out by the decreased modes $\Delta m^p_4$ along with $T^p_d$ lowing, to satisfy the SGD relation, (see in Fig.3(b) and Fig.3(c)). However, because there is higher density of phonon modes in terminal 4 than that in the symmetric situation, at initial stage, the small change of $T^p_d$ could make sufficient modes $\Delta m^p_4$ decreased to cancel out the energy input from $T^p_s$ enhance; the ratio of $\Delta m^p_1$ to $(\Delta m^p_1 + \Delta m^p_4)$ drops less with $T^p_{sd}$ increasing, in comparison with the symmetric situation. Therefore $Q_{sd}/T^p_{sd}$ increases with $T^p_{sd}$ increasing, i.e., $Q_{sd}/T^p_{sd} > 0$ and $\frac{d}{dt}(Q_{sd}/T^p_{sd}) > 0$, (see in Fig.4(d)). With $T^p_s$ increasing further, more $\Delta m^p_1$ with higher energy in terminal 1 are excited and more energy is input into system; therefore $\Delta m^p_4$ in terminal 4 reduce more and $T^p_d$ correspondingly goes much down to balance the both sides in Eq.(4). The ratio of $\Delta m^p_1$ to $(\Delta m^p_1 + \Delta m^p_4)$ decreases remarkably with $T^p_{sd}$, similar to the symmetric situation. Thus $Q_{sd}/T^p_{sd}$ changes from increase to decrease with $T^p_{sd}$, as shown in Fig.4(d); $\frac{d}{dt}(Q_{sd}/T^p_{sd}) > 0$ at beginning, and then $\frac{d}{dt}(Q_{sd}/T^p_{sd}) < 0$ after $T^p_{sd}$ passing a critical value. This means that $Q_{sd} - T^p_{sd}$ curve increases monotonously with the concave shape at beginning, and then keeps going with the convex shape after passing a turning point, and finally tends to saturation, (see in Fig.2). (ii) Thermal asymmetry and rectification discussion: in the reverse case with $T^a_d > T^a_s$, due to the higher density of phonon modes in terminal 4, $T^p_d$ enhance over $T_g$ could easily excite more $\Delta m^a_4$ in terminal 4 and makes more energy into system. This leads that $\Delta m^a_1$ in terminal 1 must decrease much, due to the larger mode spacing $\Delta = \frac{\pi v}{a_1}$ in terminal 1. Thus $T^a_s$ corresponding to $\Delta m^a_1$ decreases more, in terms of $\frac{\pi v \Delta m^a_1}{a_1} \sim k_B |T^a_s - T^a_g| / h$, (see in Fig.3(b)). The ratio of $\Delta m^a_1$ to $(\Delta m^a_1 + \Delta m^a_4)$ decreases rapidly with $T^a_{sd}$, so that $Q_{sd}$ tends more quickly to saturation in the reverse case as shown in Fig.2. Furthermore for the fixed $T_{sd}$: $|T^a_s - T^a_d| = (T^a_s - T^a_d) = (T^a_d - T^a_s) = \text{constant}$, the $\Delta m^a_1$ with higher energy for the positive case $(T^a_s > T^a_d)$ is more than the $\Delta m^a_1$ for the reverse case $(T^a_n < T^a_d)$; therefore we have $T^a_p > T^a_d$ and $T^a_p > T^a_s$, (see in Fig.3(b)). Thus, in the positive case, $T^a_s$ and $T^a_d$ locate at higher temperature region to make more modes with higher energy participated in thermal transport; for the reverse case, $T^a_s$ and $T^a_d$ is situated at lower temperature region to excite less modes with higher energy for thermal transport, (see in Fig.4(c) and Fig.3(b)). Consequently the $Q_{sd} - T_{sd}$ characteristics display a distinct asymmetry and rectifying behavior in the asymmetric structure as shown in Fig.2.
In the above discussion, the main effect of $T_g$ is to set up a reference temperature which makes the nonlinear variation of $\Delta m_1$ and $\Delta m_4$ possible.

In view of some successful thermal measurements in nanoscale\cite{3,11,12}, it is possible to realize the relevant experiments for the novel phenomena in the DFNSs. Authors think that the steady thermal flow in the ballistic system is a necessary factor to observe these thermal transiting behaviors as discussed in the paper.

In summary, thermal transistor has been designed theoretically in the DFNSs. When satisfied with the steady thermal flow condition of system, saturation and asymmetry and rectification of thermal flow are exhibited separately in the symmetric and asymmetric DFNSs. The relevant physical mechanism is elucidated by the nonlinear variation of temperature dependence of phonon modes in terminals. The mechanism is also helpful to investigation of the negative differential thermal resistance and thermal diode design in nanoscale systems.

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FIG. 1: Schematic diagrams for the research system and the working illustration of SGD. Arrow lines represent the thermal flows. (a) A four-terminal structure. (b) SGD at equilibrium: $T_s = T_g = T_d$. (c) SGD at steady state: $T_s > T_g > T_d$; a propagating channel (dash lines) is set up between the source and drain. (d) Thermal flow profile at steady state. $Q_1$ is the net thermal flow in terminal 1, and $Q^L$ is the net thermal flow across the level line (dot line) or (arrow line) in the vertical direction of region $V$ and always equals zero at steady state of system.
FIG. 2: Thermal flow $Q_{sd}$ vs temperature difference $T_{sd}$ for the gate temperature $T_g$ in the DFNS, the same structure as shown in Fig.[II]a). [Main figure] Asymmetric structure with $a_4 = 40\text{nm}$. [Inset (a)] Symmetric structure with $a_4 = 20\text{nm}$. Other parameters: $a_1 = a_2 = a_3 = 20\text{nm}$, $L = 100\text{nm}$, $b = 20\text{nm}$. 
FIG. 3: Schematic diagrams for the cutoff frequencies of discrete transverse phonon modes or threshold energy (straight lines) for terminal I, region V, and terminal IV. Dash dot dot line: the gate temperature $T_g$. Dash dot lines: temperatures $T_s$ and $T_d$. Arrow lines: the change of temperatures relative to $T_g$. The superscript $p$ represents the positive $T_{sd}$ ($T_s > T_d$); $n$ for the negative $T_{sd}$ ($T_s < T_d$). $\Delta m^p_1$ is modes in terminal 1 excited by $T^p_s$. (a) Symmetric structure. (b) Asymmetric structure for $T^p_{sd} = T^n_{sd}$.
FIG. 4: At steady state of system, for the fixed gate temperatures $T_g$: [(a) and (c)] Temperatures $T_s$ in source and $T_d$ in drain vs temperature difference $T_{sd}$ between the source and drain, respectively for the symmetric and asymmetric cases. [(b) and (d)] Thermal conductance $Q_{sd}/T_{sd}$ vs $T_{sd}$ respectively for the symmetric and asymmetric cases.