Interface thermal resistance induced by geometric shape mismatch: A multiparticle Lorentz gas model

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Poor heat dissipation caused by interface thermal resistance (ITR, or Kapitza resistance) has long been the bottleneck that limits the further miniaturization of integrated circuit. In this paper, different from previous studies on ITR induced by conjunction of two different materials, the ITR of a homogeneous stepped system is studied through the multiparticle Lorentz gas model. It is found that ITR can be triggered by pure geometric shape mismatch, and decreases when the degree of mismatch decreases. The ITRs for forward and backward transport are asymmetrical; thus, thermal rectification effect is also obtained in this system. Moreover, the effects of absolute width, width ratio, mean temperature, and temperature difference on ITR and thermal rectification effect are discussed. The ITR induced by geometric shape mismatch provides physics for interfacial thermal transport.

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I. INTRODUCTION

Integrated circuit has become the center part of a semiconductor device, which is the footstone for microelectronics and information industry. However, due to the rapidly shrinking of scale for integrated circuit, heat disposition becomes the bottleneck that limits its further development, especially when the characteristic size of the device decreases to nanoscale [1]. In this case, interface thermal resistance (ITR, or Kapitza resistance), rather than resistance of materials, dominates in thermal transport [1–4]. In addition, thermal diode and triode, which can be realized by manipulating ITR, have been proposed and become the promising thermal devices to enable better control of heat flux [5–11]. Thus, ITR is an important area worth exploring.

On one hand, different models have been put forward to understand phonon transport across interfaces, and estimate ITR [2,12]. Although great processes have been made during the past decades, present models can only deal with elastic process in a perfectly smooth or diffusive interface [1,2,12]. In this case, many numerical methods have been developed to simulate phonon transport across interfaces [1,13–15]. On the other hand, different strategies have been brought up to reduce ITR. It is found that decreasing interfacial roughness [12,16,17], introducing interlayers [18–20], and strengthening interfacial bonding [15,21–23] can effectively decrease ITR.

However, it needs to be noticed that most of previous researches are focused on interfaces formed by conjunction of different materials [1,2]. In this case, the ITR is mainly caused by mismatch of phonon spectrum between different materials [2,12]. Due to previous researches, geometric features have effective influence on particle transport [24]. It is natural that phonon transport can also be tuned by geometric shape. Actually, thermal rectification effect [25–27] and the natural graded thermal conductivity [28,29] induced by geometric shape have already been investigated. Especially, many asymmetric structures have been proposed to achieve thermal diode [5,27,30]. However, interface induced by geometric shape mismatch in a homogeneous system has not been studied yet. At the same time, a relationship between the ITR and thermal rectification effect in geometric shape mismatched structure is lacking.

In this paper, the ITR of a stepped structure madding of the same material, which consists of two rectangles with different width [shown in Fig. 1(a)], has been studied through a multiparticle Lorentz gas model. The dependence of ITR on absolute width, width ratio, mean temperature, and temperature difference is discussed. Due to the asymmetry of ITR on this system, the thermal rectification effect is found. A study about the dependence of thermal rectification ratio (TRR) on structural parameters and temperature is also performed.

II. MODELS

The Lorentz gas model, which was first proposed by Lorentz in 1905, is used to model the movement of electrons in a metallic body [31]. Recently, it has been extended by Zhang *et al.* to model phonon transport in different systems [32,33]. Generally, the model consists of particles moving with a speed depending on the temperature, which follows the Maxwell velocity distribution. Classical Lorentz gas model simulates the behavior of particles by only considering the collision of particles with boundaries of a system. In order to simulate phonon-phonon interactions which play important roles in thermal transport [1,2,15,18], the collisions between particles are considered in the multiparticle Lorentz

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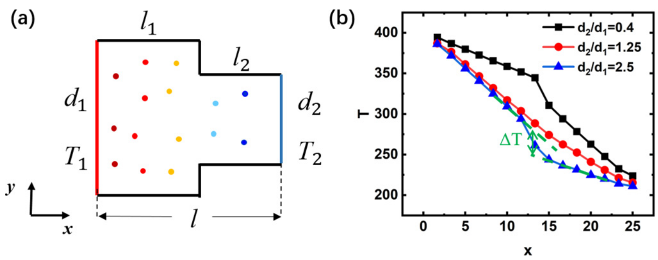

FIG. 1. (a) The modeled system with a stepped structure, which consists of two rectangles with different width. (b) Temperature distributions for systems with different width ratios (d_2/d_1). The linearly extrapolated temperature at each side of the interface is used to define the interface temperature difference (ΔT).

gas model. More details about the method can be found in previous studies by Zhang and co-workers. [10,32,33].

Our model provides an approach to investigate thermal transport. Except for materials with different geometric shapes [32], our model can realize the change of nonlinearity and category of materials conveniently by changing the collision probability and number density of particles, respectively. Thus, our model can be applied to investigate the ITR and thermal rectification effect induced by different materials and structure asymmetry or the combined effect of these two, exploring the effect of nonlinearity on thermal conductivity, ITR, and thermal rectification effect. Compared with the commonly used atomic Green's function method which can only deal with harmonic cases [34], molecular-dynamics simulation which can only deal with cases at high temperature with strong nonlinearity [1], and macroscopic continuum medium model which describes diffusive thermal transport, our model based on microscopic multiparticle statistical principle can simulate the crossover from ballistic transport to diffusive transport [5]. By setting collision probability to zero (one), ballistic (diffusive) transport can be achieved [5,35]. In this paper, using this model, we find that geometric shape mismatch can induce asymmetrical ITR. So we believe that, from another perspective, our model can contribute to the finding of new phenomena and provide understanding of mechanism for thermal transport.

The simulated stepped structure is shown in Fig. 1(a), which is composed of two rectangles with different width d_1 and d_2, respectively. Lengths of the two rectangles are l_1 and l_2, respectively. It needs to be noticed that thermal transport in similar stepped structure made of graphene has been studied previously [27,30]. However, previous studies are solely focused on thermal rectification effect. ITR of this structure has not been studied yet. What is more, ITR of the stepped structure is different from that of grain boundary which is induced by different crystalline orientation of the same material [36]. Here, there is no crystalline orientation difference in the simulated system.

In order to establish a temperature gradient, heat source of T_1 and heat sink of T_2 are applied at $x = 0$ and $x = l$, respectively. Adiabatic boundary conditions are set for all other boundaries. Therefore, when particles collide with these boundaries, only specular reflection occurs. The heat flux is calculated as Eq. (1) by counting the heat absorption and release of one heat source over a period of time. The temperature can be calculated through the kinetic energy as Eq. (2) for every particle. After obtaining the temperature distribution and heat flux, the ITR of the system can also be calculated as Eq. (3):

$$J = \frac{\Delta E}{\Delta t}, \quad E = E_{\text{released}} - E_{\text{absorbed}}, \tag{1}$$

$$T(x) = \frac{E(x)}{k_B}, \tag{2}$$

$$R = \frac{\Delta T}{J}. \tag{3}$$

Throughout this paper, dimensionless units are used; the particle mass and the Boltzmann constant k_B are set to 1.

III. RESULTS AND DISCUSSION

The temperature distributions for systems with different width ratios (d_2/d_1) are shown in Fig. 1(b). Here, T_1 and T_2 are fixed as 400 and 200, respectively. l_1 and l_2 are both fixed as 12.5. When the width ratio changes, d_2 is fixed as 10. It can be observed that there is a temperature jump at the junction part of two rectangles, which is similar to that of interfaces formed by conjunction of two different materials [18,23]. This is the signature for occurring of interfacial thermal transport, which implies that ITR is induced by geometric shape mismatch through the conjunction of two rectangles madding of same material with different widths. More importantly, the temperature jump changes when the width ratio changes. This implies that the ITR may also change.

The geometric shape mismatch-induced ITR, essentially, can be understood as analogous to the ITR by conjunction of two different materials. Generally, phonon spectrums are different for different materials. When phonons transport from one material to the other material, some of them will be scattered at the interface due to the mismatch of phonon spectrum [2]. The phonon scattering rate at the interface is different from that inside two sides of the interface. This discontinuity results in a temperature jump at the interface [1,2]. In our system, there is no phonon spectrum mismatch. However, due to the change of geometric shape, particles will experience additional scattering at the interface. This scattering is also different from the particle-particle scattering inside two sides of the interface. Thus, the discontinuity in scattering happens, and results in a temperature jump at the interface.

To better show this point, the interface temperature differences and corresponding heat fluxes under different width ratios are shown in Fig. 2(a). It can be found that the temperature difference, ΔT (black dot), gradually decreases when the width ratio increases from 0 to 1, and gradually increases when the width ratio increases from 1 to 2. That is, the greater the difference in widths between left and right rectangles, the greater the ΔT. The heat flux (red dot) keeps decreasing as the width ratio increases. Then, the ITR of different systems can be calculated through Eq. (3).

The ITRs of different systems are shown in Fig. 2(b). At first, how absolute widths of rectangles affect the ITR is studied by keeping the width ratio the same. Thus, the structure scales up when the width of the left rectangle (d_1) increases.

It can be found that when d_1 increases, the ITR stays almost the same (black dot). This point is easy to be understood. If width ratio remains the same, when the structure scales up, the number of particles increases, while the proportion of particles that scattered at the interface remains the same, which is the origin of ITR here. However, for the three lines with different width ratios, the ITR shows great difference. This implies that the width ratio, rather than the absolute width of rectangles, greatly affects ITR.

To take a step further, the ITRs for systems with different width ratios are also calculated. Here, the width of the right rectangle is fixed as 10. It can be seen from the red dot in Fig. 2(b) that when the width ratio increases to 1, the ITR decreases to 0; after then, if the width ratio increases continually, the ITR increases. That is, the bigger the difference in width between the left and right rectangle, the greater the ITR. This is because the route for particles to transport becomes narrow, particles from the heat source are easier to be scattered by boundaries at interface, and thermal transport is blocked. For the extreme condition when there is no geometric shape mismatch, no temperature jump will occur.

Subsequently, the effect of temperature on ITR is also studied. Here, the d_2 is fixed as 10. The dependence of ITR on the temperature difference of heat source and heat sink is shown in Fig. 3(a). When changing the temperature difference, the mean temperature of heat source and heat sink, $(T_1 + T_2)/2$, stays the same. This is fixed as 300. Obviously, the ITR increases silently as the interface temperature difference increases for both cases when width ratio equals 0.4 and 0.6. This is because ITR here is induced by particle scattering at boundaries of the interface. When the temperature difference increases, we keep the mean temperature the same. So, particles at the left rectangle have higher mean temperature, as well as higher energy. Particles at the right rectangle have lower energy. The thermal flux, as well as net particle transport, is from left to right. As now, particles with higher energy are scattered by boundaries at the interface, leading to less thermal energy being transported. Thus, the ITR increases.

The ITR on different mean temperatures is shown in Fig. 3(b). When changing the mean temperature, the ratio of temperature difference to mean temperature, $(T_1 - T_2)/(T_1 + T_2)$, stays the same as 1/3. It can be found that the ITR decreases as the mean temperature increases for all cases when the width ratio equals 0.4, 0.6, and 0.8. This tendency is

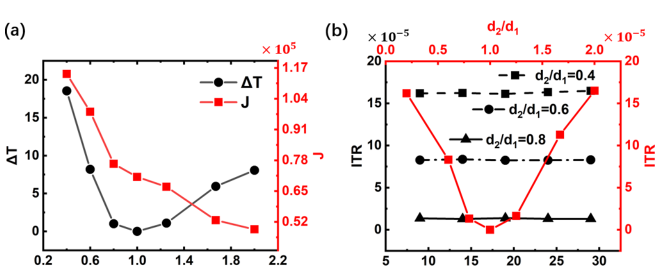

FIG. 2. (a) The dependence of interface temperature difference (ΔT, black dot) and heat flux (J, red dot) on width ratio. (b) The dependence of ITR on absolute width (d_1, black dot) and width ratio (d_2/d_1, red dot).

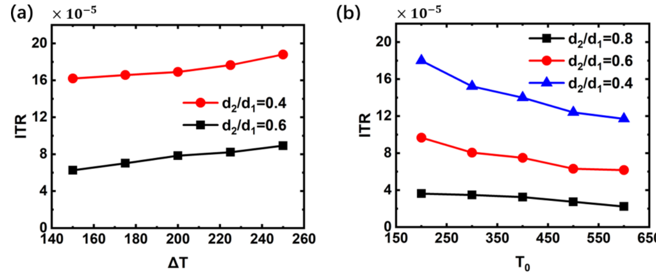

FIG. 3. (a) The dependence of ITR on temperature difference between heat source and heat sink at different width ratios (d_2/d_1). (b) The dependence of ITR on the mean temperature (T_0) of heat source and heat sink at different width ratios (d_2/d_1).

the same with results of interfaces formed by conjunction of two different materials. For the latter case, when temperature increases, the decrease of ITR is attributed to the enhancement of inelastic phonon scattering that serves as channels for thermal exchange [18,37]. Here, the results also in part come from the enhanced thermal exchange. The mean velocity of particles increases when mean temperature increases. On one hand, the collision radius stays the same when mean temperature increases. This will result in the increase of collusion for particles at unit time, which serve as channels for thermal exchange here. On the other hand, the effect of geometric shape mismatch is smeared [33], which is the origin of ITR.

An interesting phenomenon should be noticed in Fig. 2; the ITR for forward and backward transport is not equal. That is, ITR for case when the width ratio less than 1 is not in symmetry with case when the width ratio is larger than 1. For example, when the width ratio equals 0.5, the ITR is not the same as the case when the width ratio equals 2. This implies that the thermal rectification effect should exist in the system. To study the thermal rectification effect, TRR, a parameter which characterizes the intensity of thermal rectification effect, is defined as [33]

$$\gamma = \left|\frac{J_+ - J_-}{J_+ + J_-}\right|, \tag{4}$$

where J_+ is the forward heat flux when $T_1 > T_2$, and J_- is the backward heat flux when $T_1 < T_2$. Both J_+ and J_- are scalars which denote the size of heat flux. Thus, $\gamma = 0$ means that there is no thermal rectification effect, and $\gamma = 1$ means the ideal situation when there is no backward heat flux.

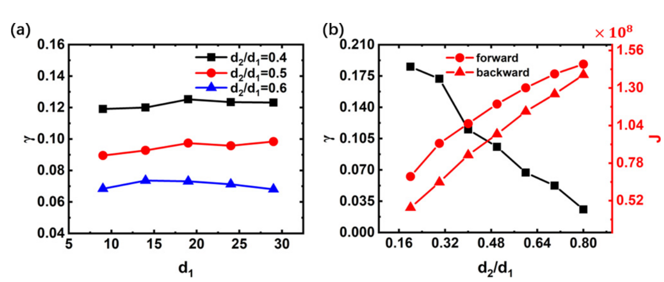

FIG. 4. (a) The dependence of TRR (γ) on absolute width of left rectangle (d_1). (b) The dependence of TRR (γ) and heat flux on width ratio (d_2/d_1).

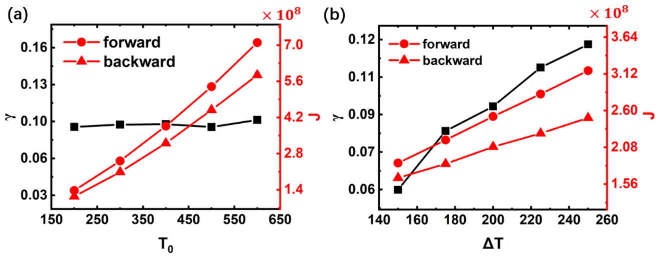

FIG. 5. The dependence of TRR (γ) and heat flux on the (a) mean temperature (T_0) and (b) temperature difference (ΔT) of heat source and heat sink.

The dependence of TRR on absolute width and width ratio is shown in Fig. 4. Similar to the situations in investigating ITR, a simple variable is kept when studying the effect of the above two factors on TRR. Here, the temperatures of heat source and heat sink are also fixed as 400 and 200, respectively. As can be seen in Fig. 4(a), the TRR is insensitive to absolute width and keeps almost the same when d_1 increases from 9 to 29 for cases when the width ratio equals 0.4, 0.5, and 0.6. However, as shown in Fig. 4(b), the TRR (black dot) decreases when the width ratio increases. This implies that the thermal rectification effect is induced by the mismatch of geometric shape. The heat fluxes along the forward and backward directions are also shown in Fig. 4(b). Heat flux along the forward direction is always larger than that along the backward direction. What is more, both the forward and the backward heat fluxes increase when the width ratio increases. This is because particle scattering at the interfaces becomes weak, and thus facilitates thermal exchange.

Another important factor that affects TRR is temperature [5,27]. The effect of mean temperature on TRR is shown in Fig. 5(a). Similar to the studying of ITR, the ratio of temperature difference to total temperature, $(T_1 - T_2)/(T_1 + T_2)$, stays the same as 1/3. It is found that the TRR (black dot) stays almost the same when the mean temperature increases from 200 to 600. In this process, both the forward and backward heat fluxes increase with mean temperature. The difference between these two shares the same increase trend as the combination of these two. Thus, the mean temperature has no effect on the TRR. The influence of temperature difference on TRR is shown in Fig. 5(b). Here, the mean temperature is fixed as $T_0 = 300$ when the temperature difference changes. The TRR (black dot) increases when the temperature difference increases. Although both forward and backward heat fluxes increase during this process, the backward heat flux grows much more slowly. Thus, the difference between these two increases faster than the combination of these two. This result is in accordance to previous researches by molecular-dynamics simulation [5,33].

It should be noticed that, generally, thermal rectification effect is induced by different temperature dependence of thermal conductivity for two materials forming the system [38], or different phonon spectra mismatch for different directions of temperature bias [5]. The latter one will result in different ITR [2]. However, our system is made of the same material; there is no phonon spectra mismatch. Previous researches have investigated the thermal rectification effect in system formed by conjunction of the same material with and without holes [38,39]. This kind of inhomogeneity is somewhat similar to our work which is induced by geometry difference. However, only the thermal rectification effect is studied, which is explained by different temperature dependence of thermal conductivity for sides with and without holes [38]. Here, we prove that the ITR is asymmetric in a system with pure geometry difference, which also can lead to the thermal rectification effect.

IV. CONCLUSION

In summary, thermal transport in a stepped structure, which consists of two rectangles madding of same material with different width is studied through the multiparticle Lorentz gas model. Due to the pure geometric shape mismatch, interface thermal resistance (ITR) exists in this homogeneous system. Due to the asymmetry of ITR for forward and backward transport, thermal rectification effect is found. It is found that the ITR and thermal rectification ratio (TRR) are insensitive to the changing of absolute width, while both increase significantly when the width ratio decreases. When mean temperature increases, the ITR decreases and TRR stays almost the same. When the temperature difference increases, the ITR silently increases and TRR hugely increases.

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