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# HEAT CONDUCTION RECTIFICATION IN NANOSTRUCTURE WITH STEP CHANGE IN CROSS-SECTION

**Xingang Liang and Bao Yue**[1]
School of Aerospace, Key Laboratory for Thermal Science and Power Engineering, Ministry of Education of China, Tsinghua University
Beijing 100084, China
[1] present address:

## ABSTRACT

Heat conduction rectifier is attracting more attention due to its potential application to process thermal currents independently and convert them into electronic signals. This work reports an investigation by molecular dynamics simulation on the heat conduction rectification effect in the nanostructure whose cross-section have step change along the heat flux. It is found that thermal resistance is different with reversed heat flux direction, which is called the heat conduction rectification. The heat conduction rectification depends on the temperature difference. By reducing temperature difference across the nanostructure, the rectification could be reversed. When the temperature difference is small enough, the thermal resistance is larger when the heat flux flows from the thick part to the thin part when the length of the structure is about 10 nm. The larger variation in the cross-section leads the larger difference in the thermal resistance with opposite heat flux. The mechanism of the rectification is discussed. If we take phonons as liquid particles and consider the case of a liquid flowing through a channel with step expansion in cross-section, the flow resistance is less with liquid flowing from the narrow part to the wide part than that in the case with contrary flow direction. In fact, the scattering of phonons at the step face reduces the mean free path of phonon when heat flux conducts from the narrow end to the wide end.

## 1 INTRODUCTION

Anisotropic thermal conductivity is popular for crystals. For example, a crystal can have different thermal conductivities in different directions because the phonon group velocities are different. For thin films the conductivities can also be different in the normal direction and the in-plane direction due to the confinement of surfaces on the phonon mean free path (MFP) (Xiao, 2004). Usually the thermal conductivity is same in one direction and does not depend on the flux direction. However, the similarity between heat conduction and electrical conduction remind us if there might be a thermal-diode or quasi-thermal-diode conduction.

Diode is a very important electronic device. It restricts current chiefly to one direction. When we exert a positive voltage over the diode, the electron can pass through it. When we put a negative bias over it no current could pass. Researchers have been seeking for thermal diodes or thermal rectifier conduction due to the similarities between electrical conductance and heat conductance (Casati, 2007; Chang, et al., 2006; Liang, 2007; Liang, et al., 2002).

For bulk materials the thermal resistance though the materials plays the dominant role in determining the thermal conductivity and the surface or interface effect is usually negligible. At microscale, however, the MFP of energy carrier is usually equivalent to the characteristic length and the interface effect could extend into the materials Liang, 2007). Interfaces have significant impacts not only on the flow and heat transfer, but also on the properties of the materials. Most of microscale phenomena result from interfaces. Many reports of experiments (Yao, 1987), theory (Chen, 1997) and molecular dynamics simulation (Feng, et al., 2001 & 2003; Liang and Sun, 2005; Liang, et al., 2006; Maiti, et al., 1997) found out that thermal conductivity is greatly reduced due to the limitation of interface on phonon transport. The interaction of an interface with an incident phonon depends on its wavelength or wavevector. The interface may produce different resistances to the phonons from the nanostructures with different density of states or different phonon wavelength regimes and result in a conduction rectification effect.

Liang et al (Liang, et al., 2002) reported a rectifier conduction phenomenon in the radial heat conduction of a nanotube of solid argon by nonequilibrium molecular dynamics simulation (MDS). The inter-atomic interaction abides by the LJ (12-6) potential. The temperature gradient across the radial direction was set up. The heat flux direction was reversed by exchanging the hot and cold regions. The thermal conductivity was determined by the Fourier law. The radial conductivity was found dependent on the heat flux direction. The conductivity obtained with heat flux from the inner to the outer surface was larger than that obtained with heat flux from the outer to the inner surface. Several factors were suggested to account for direction dependence. One was the difference in phonon spectra at the inner and the outer surfaces. The boundary requires that the minimum wave vector equal 2/d (diameter). The minimum wavevector at the inner surface is larger than that at the outer surface. When a phonon at outer surface with a wavevector out of the wavevector range at the inner surface propagates to the inner surface, it must experience a phonon collision or reflection. Thus the probability of Umklapp process is increased and a larger conduction resistance is resulted.

Recently, Liang (2007) reported a thermal rectification conduction phenomenon in the normal conduction of bi-layered nanofilm by MDS. The only different of two layers is the atom mass. It was found that the conductivity depends on the heat flux direction. When the flux was set from the layer of lighter atoms to the layer of heavier atoms, the conductivity is higher than that obtained by the reverse case. The larger difference in atom mass, the larger difference in the thermal conductivity was found. In this case, the wavevector regimes of phonons in the two layers are same because the lattice constant, layer thickness are same. However, the density of state of phonons in the two layers is different. The phonons in the layer with smaller atom mass locate in higher frequency region and have shorter wavelength and thus the interface has smaller reflection to the phonons from the layer of smaller atom mass.

Chang et al. (2006) reported a nanoscale solid-state thermal rectification. High-thermal-conductivity carbon and boron nitride nanotubes were mass-loaded externally and inhomogeneously with heavy molecules. They observed an asymmetric axial thermal conductance with greater heat flow in the direction of decreasing mass density. They suggested that solitons may be responsible for the phenomenon. Casati (2007) suggested that coating a nanotube with a molecular layer that is thicker on one end than the other could make a thermal rectifier that allows heat to flow easily along the tube in one direction, but not so easily in the opposite direction due to phonon bands mismatch in different segments.

Molecular dynamics simulation is a very effective and powerful method to investigate the heat conduction in micro/nano scale. Lukes et al. first applied molecular dynamics (MD) method to simulate the size effect of solid argon thin films and found that MD method is successful in predicting the size effect of thermal conductivity (Lukes, et al., 2000). In this paper, we report a MDS on the in-plane thermal conductivity of nanofilm with a step change of cross-section. The Ar solid and Lennard-Jones (LJ) potential which can reduce simulation times are used. The purpose is to reveal the rectification effects of step interface. If we take phonons as liquid particles and consider the case of a liquid flowing through a channel with step expansion of cross-section, the flow resistance is less than that in the case with contrary flow direction. If the analogy of the liquid flow and phonon flow do exist, the rectification of heat conduction should occur.

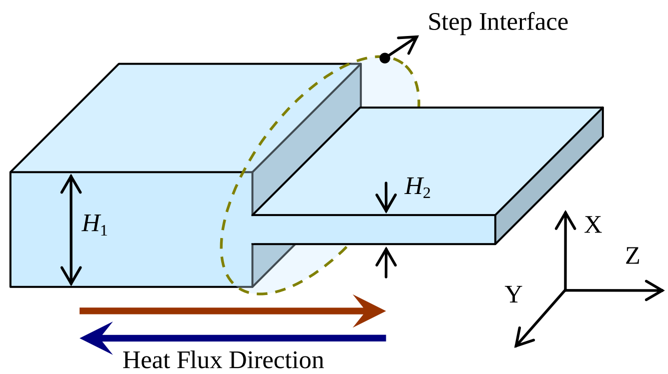


Figure 1 The schematic picture of the simulation system containing the step change in cross-section

## 2 THE SIMULATION SYSTEM

The simulation system is shown in Figure 1. The thickness of the system at each side of the step interface is $H_1$ and $H_2$ respectively, and called thick part and thin part. The total length of the system in Z direction is 21.6 nm, and the length of the thick part is equal to that of the thin part. The heat flow direction is in Z direction. The nonequilibrium simulation technique is adopted. Certain amount of heat is input in one end of the film and same amount of heat is removed at other. The heat flux direction first follows the positive Z direction and then shifts to the negative Z direction. The thermal resistance along Z direction can be obtained with different flux direction and cross-section ration, $H_1/ H_2$. The step interface effects can be observed. The system is encapsulated in a fixed adiabatic hard wall, which is composed of four layers of atoms in X and Z directions for the purpose of preventing Ar atoms from evaporating out off the system. The periodic boundary condition is applied in Y direction.

## 3 THE EFFECTS OF THE DISTRIBUTION OF TEMPERATRE

Four samples with different cross-section ratios and opposite heat flux are simulated. The ratios of thickness of the thick part to the thin part are set as I: $H_1$=1.62nm， $H_2$=1.08nm； II: $H_1$=2.16nm， $H_2$=1.08nm； III: $H_1$=2.70nm, $H_2$=1.08nm and IV: $H_1$=3.24nm， $H_2$=1.08nm. One of the typical temperature distributions is shown in Figure 2. Because the cross-section of the thick and the thin parts is different the heat flux density in the two parts and the temperature gradient are not equal. The thermal resistance is defined as:

$$R = \frac{\Delta T}{Q} \tag{1}$$

where $R$ is the thermal resistance, and the unit is K/W, $\Delta T$ is the temperature difference between two ends of the system; $Q$ is heat flux (W). Taking the cross-section ratio as the x-coordinate and the thermal resistance as the y-coordinate, the simulation results are shown in Figure 3.

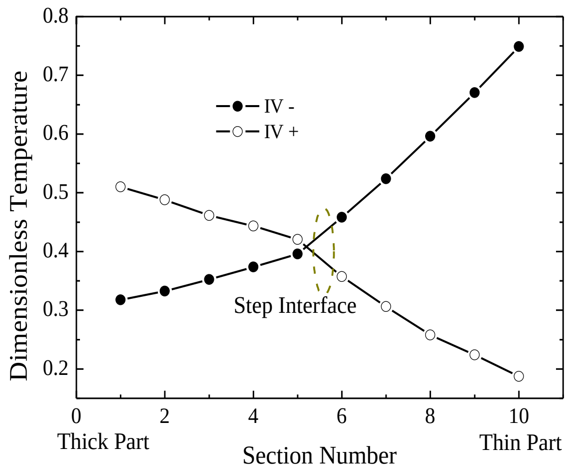


Figure 2 the system temperature distribution of sample IV in Z direction: the "+" denotes the heat flow is in the positive Z direction (from the thick part to the thin part); the "-" denotes the heat flow is along the negative Z direction (from the thin part to the thick part).

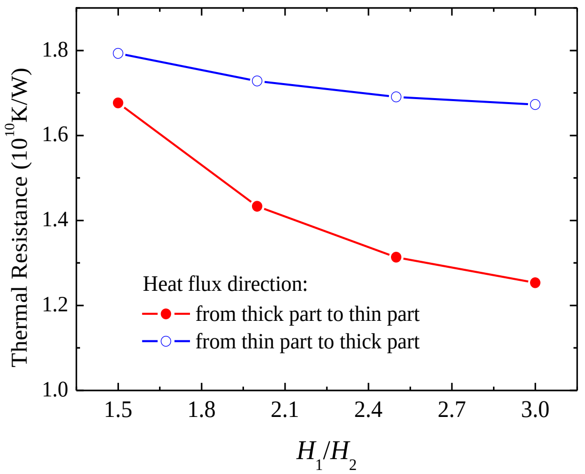


Figure 3 The thermal resistance as a function of the cross-section ratio

Figure 3 demonstrates that when the heat flux is from thick part to the thin part, the thermal resistance is smaller than the situation when the heat flux is from the thin part to the thick part. This feature is more acute with larger thickness of the thick part. This result is very hard to understand and accept. If we take the temperature distribution into account, it can be explained. The heat input is the same for the positive and negative temperature gradient in the simulation. The temperature gradient is much higher when the heat is input in the thin end, causing a higher temperature distribution as shown in Figure 2. For instance in sample IV, the temperature scale is from 22.6K to 61.7K for positive heat flux and is from 38.5 to 90.6K for negative flux. As reported by (Clayton, et al., 1973; Konstantinov, et al., 1988), the thermal conductivity of Ar is inversely proportional to temperature in the range between 20K and 90K. The same trend is also obtained in the present simulation, shown as Figure 4. When the heat flux is positive, the thermal resistance is smaller due to the lower temperature. It is hard to isolate effects of the step interface on the thermal resistance from the temperature influence. The problem is to eliminate the effects of the temperature distribution.

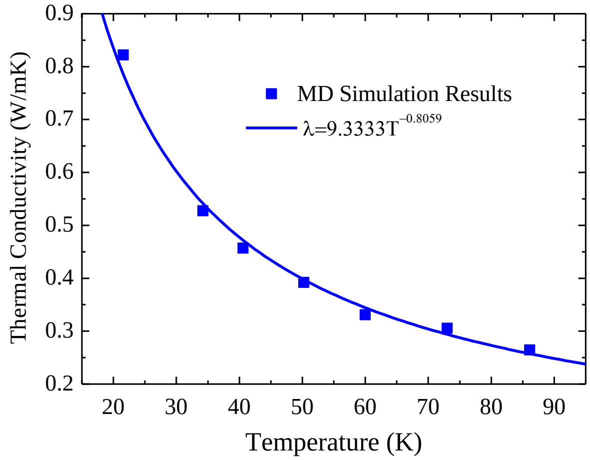


Figure 4 The thermal conductivity as a function of temperature

## 4 THE EFFECT OF THE STEP CHANGE IN CROSS-SECTION

The difference of temperature distribution under the condition of different heat flux directions produces unequal thermal resistance due to the dependence of thermal conductivity on temperature. In order to remove the influence of temperature, three steps are taken. 1) The system temperature is set at about 75K at which the influence of temperature on the thermal conductivity comparatively smoothly (Figure 4); 2) The input heat flux is decreased. According to the Fourier principle, the temperature gradient will decrease and the range of temperature distribution is reduced; 3) The length of the system is cut down, then the scale of temperature distribution is reduced. And also it is enhanced the collision of phonons

Table 1 The scales of temperature distributions of three samples

| Direction of heat flux | A（K） | B（K） | C（K） |
| --- | --- | --- | --- |
| From thick part to thin part | 71.2-79.1 | 67.9-79.3 | 64.6-78.8 |
| From thin part to thick part | 73.6-81.5 | 73.8- 84.7 | 73.4-86.2 |

emitted from the heating sector against step interface and makes the step change of cross-section interface effects more significant.

Three samples with different heat flux direction are investigated. The thickness of the samples is: A: $H_1$=2.16nm, $H_2$=1.08nm； B： $H_1$=3.24nm, $H_2$=1.08nm； C： $H_1$=3.79nm, $H_2$=1.08nm, respectively. The length of these samples is 10.8 nm, and the length of the thick and thin part is 5.4 nm, respectively. The scales of the temperature distributions are listed table 1 and is found narrowed.

Figure 5 shows the variation of the thermal resistance with the cross-section ratio at different heat flux directions. It is found that when the heat flux is positive, the thermal resistance is bigger than the situation of negative flux, and with the increase of the thickness of the thick part the contrast is more acute.

The ranges of temperature distribution with different heat flux directions are reduced indeed as shown in table 1. However, the average temperature is still lower for the positive heat flux than the negative, and thus reduces the thermal resistance in the positive direction.

Only in the case that the temperature ranges and levels are kept the same for the positive and negative heat flux the step interface effect can be fully recognized. The quantity of heat input and the average temperature are further adjusted so that the scale of temperature of samples A, B and C is almost identical at different flux directions. The temperature scales is listed in Table 2. The system thermal resistance is shown in the Figure 6. The same trend is found as that in Figure 5 and the difference in the thermal resistance is even more significant.

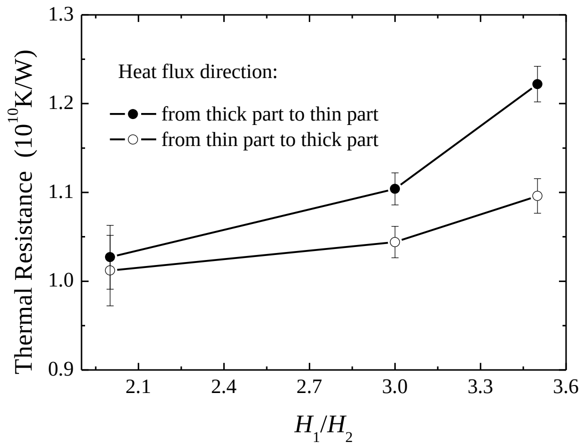


Figure 5 The thermal resistance as a function of the cross-section ratio with narrow temperature difference

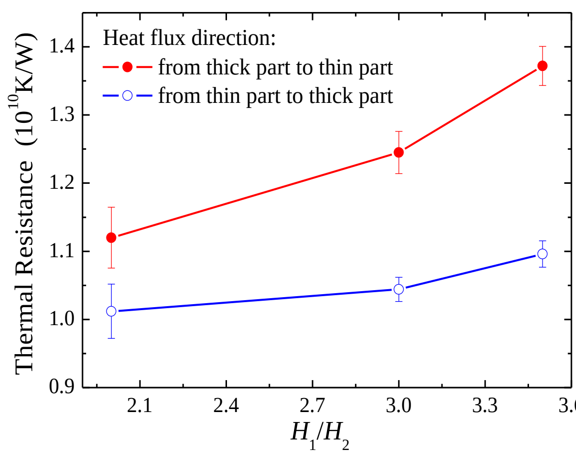


Figure 6 The thermal resistance as a function of the cross-section ratio (keeping same temperature scale and level for the positive and negative flux)

The effect of the step interface on thermal resistance is a novel observation. No such report is found by the authors' and

Table 2 the temperature distribution

| Direction of heat flux | A（K） | B（K） | C（K） |
| --- | --- | --- | --- |
| From thick part to thin part (Scale of temperature distribution) | 73.28-83.11 | 73.47-84.22 | 72.47-84.76 |
| From thin part to thick part (Scale of temperature distribution) | 73.63-81.49 | 73.85- 84.66 | 73.45-86.23 |
| From thick part to thin part (average temperature) | 78.60 | 80.97 | 81.47 |
| From thin part to thick part (average temperature) | 76.30 | 76.24 | 76.24 |

there is no quantificational model to describe its effects. The authors could only give a qualitative explanation from the phonon scattering theory here. Phonon is the quantized lattice vibration and it is the major heat carriers in solid argon. When a phonon hits an interface there are two kinds of reflection, diffuse reflection and specular reflection. As we know, the thermal conductivity, $k$, is related to the mean free path (MFP) of phonons, $l$,

$$k = cvl/3 \tag{2}$$

where $c$ is the volumetric specific heat and $v$ is the phonon group velocity. At microscale, the collision with the interface will restrict and reduce the MFP of phonons. When the heat flux is from thick part to the thin part, a large number of phonons will collide with the step interface and the MFP of phonons is shorter. According to the formula (1), the thermal conductivity is smaller and thus the thermal resistance is larger.

## ACKNOWLEDGMENTS

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