# Thermal Transport Through 1D Sandwich Structure

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**Abstract.** In present paper we proposed 1D sandwich model to investigate heat transport. Basically, sandwich model consists of three regions in which the middle region is filled with different material than that of two outer regions. We simulated temperature profile, heat flux and thermal conductivity of one dimensional sandwich structure as a function of thickness of filling part of the model. The interface thermal resistance and temperature gradient are also computed. FPU-β potential is used as intermolecular potential. The outer layers of the sandwich structure are kept at constant temperature $T_L$ = 1.1 and $T_R$ = 0.9 using Langevin heat baths. The mass of each oscillators in outer layer is taken as M = 1.0 while that in the filler layer is $M_s$ = 0.5. It is noticed that as the thickness of sandwiched layer increases, the heat flux and hence the thermal conductivity increases. The phonon propagation from left layer to middle layer (from higher mass to lower mass) and again from middle layer to right layer (from lower mass to again higher mass) is found less thermal resistive in the present case. In this case, the distance between two interfaces plays very important role in overall performance of the sandwich model. The model can be used to design good thermal conductor or insulator by varying width of the filler layer.

**Keywords:** Sandwich Model, Interface Thermal Resistance, Temperature Gradient, Heat flux, Thermal Conductivity

## I. INTRODUCTION

It is known that the thermal interfacial materials (fillers) like nano tubes, nano rods and nano wires are used as connectors or to prevent the direct connection of system to heat source/heat sink in many types of thermoelectric device [1-3]. The choice of these fillers affects the conductivity through dissimilar interfaces of the devices. Here, 1D sandwich model is proposed to investigate heat transport at low dimensions. The sandwich model consists of three regions in which the middle region is filled with different material than that of two outer regions.As we talk about thermal transport at low dimension, it is also known that the thermal conductivity is greatly depends on the size of the thermal device [4-12]. In present study, we reported the size-effect of the filler segment, which connects two phonon channels of same type. The interface between middle (filler) region and the outer region (left and right) produces the effective thermal resistance called as interface thermal resistance (ITR) or Kapitza resistance [7,14]. Hence, matching or mismatching of the Kapitza resistance affect the flow of heat from one end to another end [7,13,14]. In the present study, the total length of the sandwich model is kept fix and by varying the size of the filler layer, temperature profile, heat flux, ITR, and thermal conductivity are studied.

Contributed Paper

## II. MODEL AND METHODOLOGY

The schematic representation of one dimensional sandwich model is shown in Figure 1.

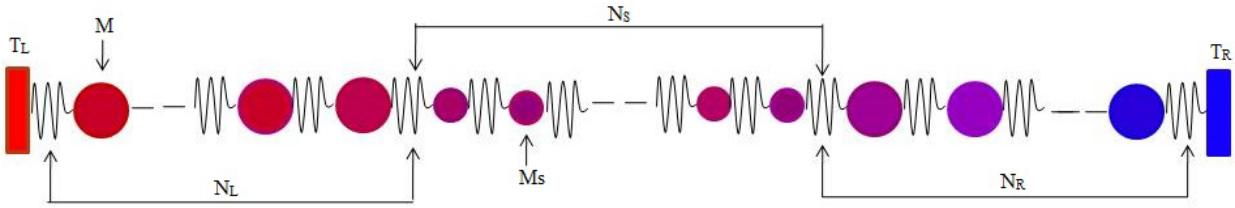



**FIGURE 1.**The schematic diagram of the one dimensional sandwich model.

The Hamiltonian for this one dimensional sandwich chain is written as [7, 13, 14],

$$H = \sum\left[\frac{p_i^2}{2M_i} + V(x_i - x_{i-1})\right]; \text{ Where } V(x_i - x_{i-1}) = \frac{K}{2}(x_i - x_{i-1})^2 + \frac{\beta}{4}(x_i - x_{i-1})^4 \quad (1)$$

Here, $p_i$ and $M_i$ are the momentum and mass of the i$^{th}$ particle, respectively. $V(x_i - x_{i-1})$is interaction potential between nearest neighbors. $x_i$ and $x_{i-1}$ gives the position of the i$^{th}$ and (i-1)$^{th}$ particles, respectively. In our simulation work FPU-β model is used to describe intermolecular potential. $K$ is the spring constant and $\beta$ is the anharmonicity parameter of the potential. As taken in our earlier paper, we kept $K$ = 1 and $\beta$ = 1 [7]. The mass of each oscillator in outer layers is taken as $M_i$ = $M$= 1 and for filler (sandwich) layer $M_i$ = $M_s$= 0.5. For the present study, the system size, i.e, the number of oscillators in Left ($N_L$), Sandwich ($N_s$), and Right ($N_R$)segments is taken as $N$ = $N_L$+ $Ns$ + $N_R$ =220.The Stochastic - Langevin heat baths are used to maintain constant temperature on the two ends with the fixed boundary condition. The temperature maintained at the first oscillator (left hand side) and the last oscillator (right hand side) are $T_L$ = 1.1 and $T_R$ = 0.9, respectively. All the parameters used are in dimensionless unit and as per the general notations.

The equations of motion of system in thermal contact with Langevin heat bath are given as [7]:

$$M_1 \ddot{x}_1 = F_1 - F_2 - \left(\xi_L - \lambda_L \dot{x}_1\right) \quad (2)$$

$$M_N \ddot{x}_N = F_N - F_{N+1} - \left(\xi_R - \lambda_R \dot{x}_N\right) \quad (3)$$

$$M_i \ddot{x}_i = F_i - F_{i+1} \quad \text{for } i = 2, 3\text{.....}, \text{N-1} \quad (4)$$

Here, as per the definition of force $F = (-\partial V / \partial x)$, $\xi$ is an independent wiener process with zero mean and $\lambda$ =1 [7, 14]. We used the seventh order Runge - Kutta algorithm to solve the differential equation. This Non-Equilibrium Molecular Dynamics Simulation (NEMDS) have been performed for >$10^7$ times so that our systems reaches to a non-equilibrium steady state.
The continuity equation relates the energy density $\varepsilon(x,t)$ and heat flux $j(x,t)$ is:

$$\frac{\partial \varepsilon(x,t)}{\partial t} + \frac{\partial j(x,t)}{\partial x} = 0 \tag{5}$$

The energy density for instantaneous position *i* is given as:

$$\varepsilon_i = \frac{p_i^2}{2m_i} + \frac{1}{2}[V(x_{i+1} - x_i) + V(x_i - x_{i-1})] \tag{6}$$

$$\therefore \frac{\partial \varepsilon_i}{\partial t} = m_i \dot{x}_i \ddot{x}_i - \frac{1}{2}[(\dot{x}_{i+1} - \dot{x}_i)F(x_{i+1} - x_i) + (\dot{x}_i - \dot{x}_{i-1})F(x_i - x_{i-1})] \tag{7}$$

On substituting $m_i \ddot{x}_i = F(x_i - x_{i-1}) - F(x_{i+1} - x_i)$ we get:

$$\frac{\partial \varepsilon_i}{\partial t} = -\frac{1}{2}[(\dot{x}_{i+1} + \dot{x}_i)F(x_{i+1} - x_i) - (\dot{x}_i + \dot{x}_{i-1})F(x_i - x_{i-1})] \tag{8}$$

Hence by comparing this equation with continuity equation we have local heat flux at *i* as:

$$j_i = \dot{x}_i \frac{\partial V(x_i - x_{i-1})}{\partial x_i} \tag{9}$$

Finally, the thermal conductivity κ and ITR is computed by [7, 13, 14]:

$$\kappa = \frac{-J}{\partial T/\partial x} \text{ and } ITR = \frac{\Delta T}{J} \tag{10}$$

Here, $\Delta T$ is the temperature drop at the interface and *J* is the average heat flux of the sandwich structure.

## III. RESULTS AND DISCUSSION

In present non equilibrium molecular dynamics simulation, the temperature profile, thermal conductivity and heat flux are simulated as a function of the thickness of the middle region. Total number of oscillators of the sandwich structure is $N = N_L+N_S+N_R = 220$. Various simulation experiments were carried out for different combinations of outer region and filler region thickness such as (100+20+100), (90+40+90), (80+60+80), (70+80+70), (60+100+60), (50+120+50), (40+140+40), (30+160+30) and (20+180+20).The temperature profiles of present models are as shown in Figure 2. An abrupt temperature drop at the junction between two dissimilar materials is clearly seen, which is the signature of an ITR. The temperature gradient of the middle segment is smaller than that of the outer layers in the present cases. It is also observed that the temperature gradient of the left segment attached with higher temperature bath is higher than the right segment attached to the lower temperature bath. ITR for the first interface is lower than that of the second interface. This is because of phonon propagates from higher mass to lower mass at the first interface, and at the second interface the phonon transfer is from lower mass to higher mass. The heat flux and the thermal conductivity simulated are shown in Figures 3(a) and 3(b) respectively. For the present 1D sandwich models, the heat flux and the thermal conductivity follows cubic relation as a function of filler size. Thus, present study reveals that the thermal conductivity can be tuned as a function of the size of the filler material. Hence, present process of simulation is helpful in designing the materials with desired thermal conductivity.

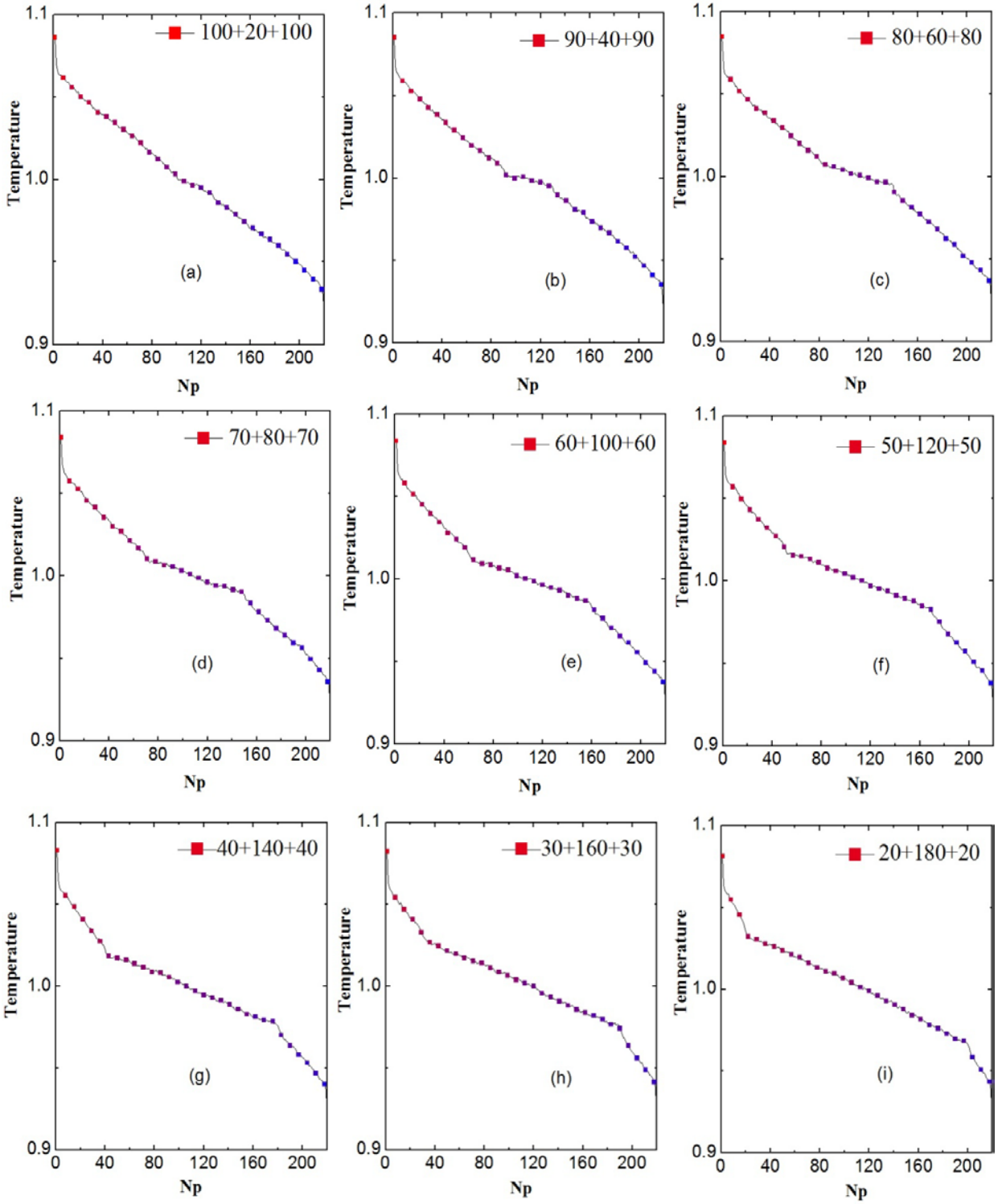
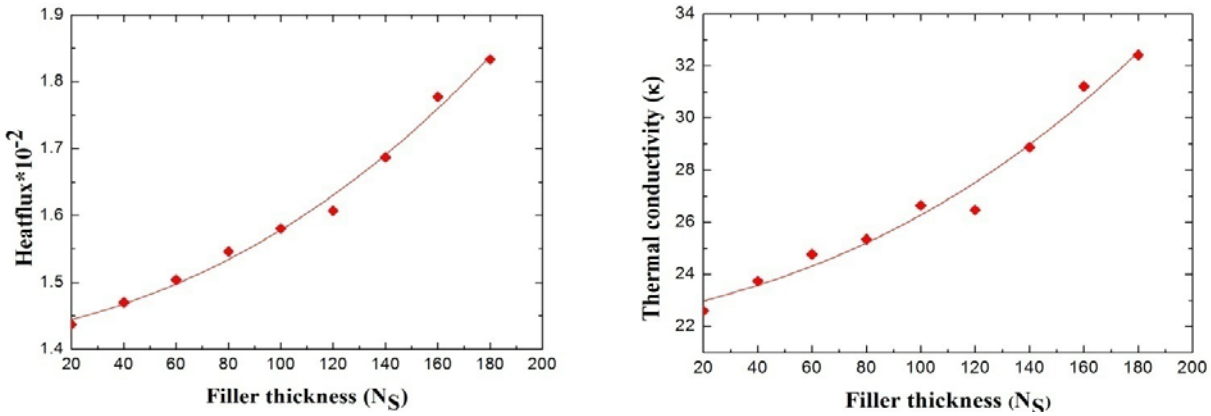



**FIGURE 2.**Temperature profile for 1D sandwich structures. The system size $N = N_L+N_S+N_R = 220$. (a)100+20+100 (b)90+40+90 (c)80+60+80 (d)70+80+70 (e)60+100+60 (f)50+120+50 (g)40+140+40 (h)30+160+30 (i)20+180+20, $T_L$ =1.1, $T_R$ =0.9, $M_L = M_R$ =1, $M_s$ = 0.5.




(a) (b)

**FIGURE3.** (a) Heat flux and (b) Thermal conductivity as a function of filler thickness. Line drawn is just to guide our eyes.

## IV. CONCLUSION

The interface thermal resistance is observed at the junction of two dissimilar materials. The thickness of the filler layer leads to decreases the temperature gradient of the filler layer as well as outer layers and hence it enhances the overall heat flux and thermal conductivity of sandwich model. It is concluded the heat flux and thermal conductivity is increases as a cubic function of the filler thickness for the present structures. Thus, this model is very helpful to design a good thermal conducting device with desire thermal conductivity.

## ACKNOWLEDGEMENT

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