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Interface thermal resistance and thermal conductivity in composites – an abrupt junction thermal diode model

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ABSTRACT

An abrupt junction diode model is proposed to study the interface thermal resistance and thermal conductivity of composite. We have demonstrated that the structure of thermal diode greatly influences the heat flow and hence it is possible to regulate the heat flow via the geometry of the diode. The composite materials can significantly reduce the thermal conductivity compared to an equivalent single material. By tuning the mass ratio of oscillator of right segment to that of oscillator of left segment of the composite, M_R/M_L, crossover between negative differential thermal resistance and positive differential thermal resistance as well as figure of merit for composite material can be tuned. It is also seen that the composite will work as a better thermal insulating material than its pure constituent materials.

1. Introduction

During last decade, investigations on thermal transport have made eye-catching progress [1–4]. Researchers in the field have studied temperature profile, rectification of heat flux, interface thermal resistance, negative differential thermal resistance, and thermal efficiency for various structures [5–30]. The main emphases of these studies remain two-fold: one to establish a convincing mechanism to explain thermal conductivity at low-dimensions and second is to make thermal devices for efficient use of phononic flow.

Many attempts have been reported to understand the mechanism of the Fourier law of heat conduction at low dimension which results in variety of features [1–30]. These features are very much important in energy transport through heat in nano-tubes, nano-wires, nano-horns, nano-cones, nano-ribbons, nano-channels [5–14]. Scientific outcomes have opened the possibility of realizing thermal devices like thermal rectifier, thermal diode, thermal transistor, thermal logic gates, thermal memory, acoustic diode, revere diode, functional graded materials, quantum structures and networks [15–30]. Scientists in the field now realized that, if heat flow in materials could be controlled then variety of innovations could occur in thermal management. Terraneo et al. [15] have proposed first prototype three segment sandwich model of thermal rectifier using 1D chain with Morse on-site potential. On the match–mismatch of effective phonon theory Li et al. [16] have constructed 1D thermal diode by coupling two FK chains of different spring constants coupled with weak harmonic spring. Later Li et al. [17] proposed an improved model of thermal diode with one segment of FK chain and second segment of FPU-β chain. These two segments are connected through a weak harmonic spring constant. Reversal of rectification in two-segment FK model is shown by Hu et al. [18]. All these reports have motivated us to undertake the study on thermal properties of composite of two dissimilar mass segments, namely, 1D abrupt junction thermal diode. Each segment of newly proposed composite – abrupt junction thermal diode is made up of Fermi–Pasta–Ulma-β (FPU-β) chain [25,26,31], each oscillator of left segment is of mass M_L and that of right segment is of mass M_R (Fig. 1). In an electronic diode, the size of p-type or n-type region as well as doping in these regions plays an important role in its performance. Hence, the purpose of the present study is to investigate: (i) temperature profile, heat flux, thermal conductivity, and interface thermal resistance (ITR) as a function of the size of diode segments; and (ii) heat flux and interface thermal resistance (ITR) as a function of mass ratio M_R/M_L.

2. Methodology

The model shown in Fig. 1, consists of two FPU-β chains. All oscillators are align along the chain stationarily with equal

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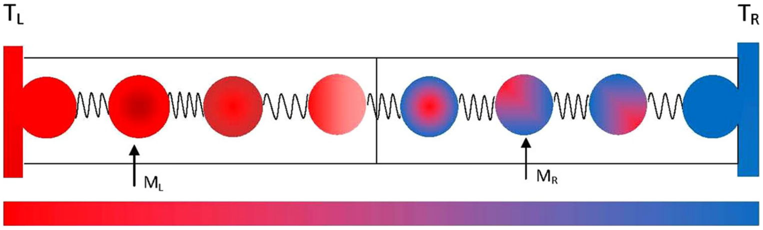

Fig. 1. Pictorial representation of 1D abrupt junction thermal diode. Each oscillator of left segment is of mass M_L and that of right segment is of M_R. $T_L > T_R$.

distance a. The Hamiltonian of composite made up of two dissimilar mass segment chains is,

$$H = H_L + H_R \tag{1}$$

where H_L and H_R are the Hamiltonian of the FPU-β model with appropriate parameters for the left segment and the right segment, respectively, of the diode:

$$H_{L,R} = \sum_i \frac{p_i^2}{2M_{L,R}} + V_{FPU\text{-}\beta}(x_{i-1}, x_i) \tag{2}$$

$$H_{L,R} = \sum_i \frac{p_i^2}{2M_{L,R}} + k\left[\frac{1}{2}(x_i - x_{i-1} - a)^2 + \frac{\beta}{4}(x_i - x_{i-1} - a)^4\right] \tag{3}$$

Here x_i is the position of each the ith particle along the chain, a is the equilibrium distance among nearest neighbors, β is an anharmonicity parameter, k is the spring constant, $M_{L,R}$ is the mass of respective particle. The term $(x_i - x_{i-1} - a)$ is the deviation from the equilibrium distance between nearest neighbors.

The Langevin heat baths are put on the first (left) and the last (right) particles [1,4,25,26] of the composite to keep temperature constant at T_L and T_R, respectively. The equation of motion of the two particles connected with Langevin heat baths are:

$$M_1\ddot{x}_1 = F_1 - F_2 - (\xi_L - \lambda_L\dot{x}_1), \tag{4}$$

$$M_N\ddot{x}_N = F_N - F_{N+1} - (\xi_R - \lambda_R\dot{x}_N). \tag{5}$$

The equations of motion for the particles between two heat baths are:

$$M_i\ddot{x}_i = F_i - F_{i+1}, \quad \text{for } i = 2 \text{ to } N-1. \tag{6}$$

With $M_i = M_L$ for $i = 2$ to $N/2$ (for left segment), and $M_i = M_R$ for $i = N/2 + 1$ to $N - 1$ (for right segment).

Here $F_i = -\partial H/\partial x_i$ is the force and $\lambda_{L,R}$ is variance parameter. The $\xi_{L,R}$ is an independent Wiener process with zero mean related to the usual fluctuation–dissipation relations [1,4]:

$$\left\langle \xi_L(t)\xi_L(t')\right\rangle = 2k_B T_L \delta(t - t')$$

$$\left\langle \xi_R(t)\xi_R(t')\right\rangle = 2k_B T_R \delta(t - t')$$

$$\left\langle \xi_L(t)\xi_R(t')\right\rangle = 0$$

The $\xi_{L,R}$ and variance parameter $\lambda_{L,R}$ which models the microscopic action of the thermostats and implement the interaction of the first and last particles with the heat reservoirs by introducing random forces and dissipation [1,4,25,26].

The local heat flux at site i is simulated by

$$J_i = \frac{1}{2}a\left\langle (\dot{x}_{i+1} + \dot{x}_i)F(x_{i+1} - x_i)\right\rangle. \tag{7}$$

When the system reaches to non-equilibrium steady state with local thermal equilibrium, J_i is independent of the index i and finally the thermal conductivity is computed by

$$\kappa = \frac{-J}{dT/dx}. \tag{8}$$

When heat current passes through an interface between two different materials there exist a temperature jump at interface from which an interface thermal resistance (ITR) is defined as [30,32]

$$R = \frac{\Delta T}{J} \tag{9}$$

Here ΔT is the temperature drop at the interface and J is the heat flux flowing through interface.

In our simulation works, seventh order Runge–Kutta method is used to solve these non-linear dynamics situation along with fixed boundary conditions. Extensive simulations have been performed for $t > 10^7$ time steps so that system attends a non-equilibrium steady state. As per the convention, dimensionless units for mass, temperature, heat flux, ITR and thermal conductivity are considered. We have used fixed boundary condition with $T_L = 1.1$ and $T_R = 0.9$, variance parameter $\lambda_L = \lambda_R = 1$, anharmonicity parameter $\beta = 1$, coupling constants $k = k_{int} = 1$, lattice constant $a = 1$.

3. Results and discussion

3.1. Size effect

Before fabricating composites, simulations are performed on pure materials. First simulations have been carried out for two FPU-β chains: (i) 1D chain of 100 oscillators with each oscillator of mass $M = 0.1$ and (ii) 1D chain of 100 oscillators with each oscillator of mass $M = 1$. Fig. 2 shows computed temperature profiles for these two 1D chains. It is seen that for chain-(i) consisting each oscillator of mass $M = 0.1$, the temperature gradient is less compared to that of the chain-(ii) consisting each oscillator of mass $M = 1$. The heat fluxes obtained for these two chains are: (i) $J(M = 0.1) = 4.32 \times 10^{-2}$ and (ii) $J(M = 1) = 2.08 \times 10^{-2}$. The thermal conductivities for corresponding chains are $\kappa(M = 0.1) = 49.3734$ and $\kappa(M = 1) = 18.4234$. The reason for the thermal conductivity of lighter lattice is higher than the thermal conductivity of denser lattice, $\kappa(M = 0.1) > \kappa(M = 1)$ is that the phonon traveling in a denser lattice suffers higher thermal resistance than the phonon traveling through lighter lattice.

The composite–abrupt junction thermal diode is made by combining two materials having oscillators of different mass. In present model, the left segment of diode consists of N_L oscillators each of mass $M_L = 1$ and the right segment of the diode consists of N_R oscillators each of mass $M_R = 0.1$. To investigate segment's size effect on the thermal transport in 1D abrupt junction thermal diode, here we have considered nine different thermal diodes with number of oscillators in left and right segment varies as N_L:N_R = 10:90, 20:80, 30:70, 40:60, 50:50, 60:40, 70:30, 80:20, and 90:10, keeping total number of oscillators in present diode model as $N = N_L + N_R = 100$. The left end (first) particle of the thermal diode is kept at constant temperature $T_L = 1.1$ and the right end (last) particle of the thermal diode is kept at constant temperature $T_R = 0.9$. Extensive molecular dynamics simulations have been performed for $t > 10^7$ time units so that system attends a stationary state and the local heat flux is become constant along the chain. Thus simulated temperature profiles for above