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Heat Transport in One-dimensional Dimer Chain

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The thermal transport phenomenon through one-dimensional dimer chain is important for the development of a new generation of small-scale thermal devices. The heat conduction in one-dimensional two component (dimer like) structures is studied using Non Equilibrium Molecular Dynamics Simulation (NEMDS). The dimers like AB .... BA and BA .... AB are considered in the present study. We have taken total 11 layers in the structure and the each layer has 20 oscillators in it. The number of total oscillators of the whole chain is $N = 220$. The extreme ends of the dimer chains are connected with Langevin heat bath to keep constant temperature on both ends. The FPU-β potential is used to calculate the intermolecular potential with $\beta = 1$. The temperature profile, heat flux and thermal conductivity are studied as functions of mass of an oscillator M_B (0.1, 0.2 ... 0.8, 0.9) in layer B. The mass of each oscillator in layer A is kept constant as $M_A = 1.0$, where $M_B < M_A$. The temperature gradient and interface thermal resistance at each interface are calculated for both dimer structures. The increase in mass of an oscillator of layer B leads to an increase in heat flux and thermal conductivity of the structures. It is observed that the ABABABABABA structure is more heat conductive structure than the BABABABABAB structure. Thus, ABABABABABA dimer is better thermal conductor while BABABABABAB dimer is better thermoelectric material.

Keywords: Heat conduction, Interface thermal resistance, Thermal conductivity, Dimer chain, Thermoelectric materials.

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1. INTRODUCTION

The major technical problem, which deteriorates the performance of nanoscale devices, is the production of unwanted heat during its operation. When the size of the structure decreases, the heat dissipation increases and hence directly affects the efficiency as well as the performance of the device [1, 2]. To drag radiant heat we need good heat sinking materials, which absorb the heat very rapidly. On the other hand, the material with low thermal conductivity is a desired feature for thermoelectric systems [3-6]. Thus, without understanding detail dynamics of heat carrier- "*phonon*", it is not possible to make modifications in materials structures for their fruitful use [7-9]. Such study is helpful to design materials for thermal applications like heat pump, heat exchanger, thermoelectric generator, thermal moderator of nanoscale. Many researches have been done on multilayered structures, which demonstrated the tuning of thermal conductivity [4-6, 10-16]. Going on step ahead, in the present study, we investigated the response of phononic flow in one-dimensional multilayered dimer chains. Basically, a dimer chain is a multilayered structure, in which two different types of materials are arranged alternatively. Hence in dimer chain, stacking of materials A and B is like ABAB.....ABA or BABA.....BAB. In the dimer, due to the two types of materials are arranged alternatingly, number of interfaces present affects their thermal response. In general, the non-zero interface thermal resistance (ITR) is produced at the interface of two materials of different masses [17-20]. In the present case, we took the mass of an oscillator of material A as M_A and that of an oscillator of material B as M_B. The mass mismatch between material A and material B at the interface in a dimer chain is the key of controlling the phonon scattering rate. In such chains, phonons with a certain frequency range only can pass through neighboring layers due to mass mismatch of the structures [9]. The thermal conductivity is reduced in such structures due to the suppression of the phonons of certain frequencies at different interfaces of the structures. There are many reports on layered structures, where the reduction in the thermal conductivity is observed for different semiconductor materials like Si/Ge [7-9, 13], Kr/Ar [16], and GaAs/AlAs [11].

With this, in the present work, we have taken two types of one-dimensional multilayered dimer chains: (i) ABABABABABA and (ii) BABABABABAB; made up by the use of two different materials A and B. The mass of an oscillator of the material A is taken as M_A and the mass of an oscillator of the material B is taken as M_B. The non-equilibrium molecular dynamics simulation (NEMDS) has been carried out to study the thermal transfer through one-dimensional dimer. The total number of oscillators in both types of one-dimensional multilayered dimer chains viz. ABABABABABA and BABABABABAB is $N = 220$, in which each block of A and B contains 20 oscillators. As the dimer chain contains 11 layers of two different materials A and B, there exist total 10 interfaces in the one-dimensional structure. The schematic representation of the chains is shown in Fig. 1. Here the left end of the dimer chain is connected to the hot temperature bath and the right one to the cold temperature bath. The Langevin heat baths are used in the present work. In the present simulation study, the effect of M_B on the heat conduction in the mentioned two types of dimer structures is

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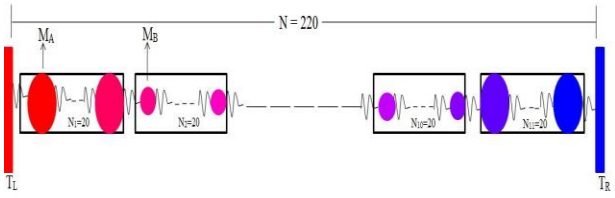
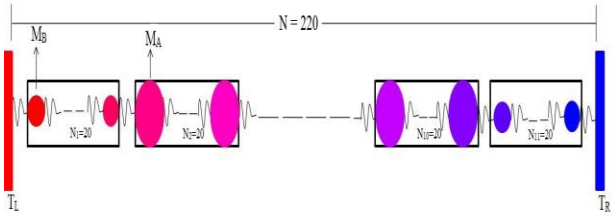
investigated. The mass mismatch of material constituents A and B in the dimer chain leads to different cut off frequencies and density of states of phonons. The differences in cut off frequencies oppose the phonon flow and generate non-zero resistance to the phonons at the interfaces [17, 18]. Due to the ITR produced at each interface of the chain, large reduction in heat flux and thermal conductivity is observed when phonons move from hot end to cold end. We simulated the temperature profile, heat flux, ITR and thermal conductivity of various dimer chains.



a



b

Fig. 1 – Schematic daigram of ABAB…..ABA (a), BABA….BAB (b) dimer chains

2. METHOD OF COMPUTATION

To express the interaction among the nearest neighbors, we have considered most commonly adopted FPU-β model. The Hamiltonian of one-dimensional dimer chain is given by

$$H = \sum_i \left[\frac{P_i^2}{2M_i} + V_{FPU-\beta} \right],$$

where, P_i is the momentum of i^{th} particle, M_i is the mass of i^{th} oscillator, $M_i = M_A$ for the mass of oscillators for material A and $M_i = M_B$ for the mass of oscillators for material B. The interaction potential is [19, 20]

$$V_{FPU-\beta} = \frac{K}{2}(q_i - q_{i-1} - a)^2 + \frac{\beta}{2}(q_i - q_{i-1} - a)^4.$$

In above equation, a is the lattice constant, q_i is the position of the i^{th} particle, K is the spring constant, and β is the anharmonicity parameter. In the present simulation, we took $a = 1$, $K = 1$ and $\beta = 1.0$. We fixed the temperature on the first particle of the chain at $T_L = 1.1$ and on the last particle of the chain at $T_R = 0.9$ by Langevin heat baths. We also applied fixed boundary conditions.

The motion between oscillators is due to the Langevin heat bath, which provides the constant temperature between the first and last oscillators of the chain. The equation of motion of the dimer chain is given as [19]

$$M_i \ddot{q}_i = F_i - F_{i+1} - (\xi_L - \lambda_L \dot{q}_i)\delta_{i,1} - (\xi_R - \lambda_R \dot{q}_N)\delta_{i,N}.$$

In above equation, $\lambda_{L,R}$ is the variance parameter, $F_i = -\frac{\partial H}{\partial q_i}$ is the force on the i^{th} particle. $\xi_{L,R}$ and variance parameter show the microscopic action of heat bath and it executes interaction of the first and last particles with thermal reservoirs. It also includes random forces and dissipation. $\xi_{L,R}$ is an independent Wiener process with zero mean concerned with the usual fluctuation dissipation relations as [19]:

$$\langle \xi_L(t)\xi_L(t') \rangle = 2K_B T_L \delta(t - t'),$$

$$\langle \xi_R(t)\xi_R(t') \rangle = 2K_B T_R \delta(t - t').$$

The local heat flux is generated by [19, 20],

$$J_i = \dot{q}_i \frac{\partial V(q_{i-1}, q_i)}{\partial q_i}.$$

The 7$^{\text{th}}$-order Runge-Kutta algorithm is used with fixed boundary conditions to perform NEMDS. We performed this simulation for > 10^7 times such as the system reaches the non-equilibrium thermal steady state condition. For such a long simulation, J_i is independent of the index i and hence the thermal conductivity is computed by [19, 20],

$$\kappa = \frac{-J}{dT/dq}.$$

Here, dT/dq is a temperature gradient in the chain.

When the phonon propagates through the interface, the produced interface thermal resistance is calculated by [17, 18],

$$R = \frac{dT/dq}{J}.$$

3. RESULTS AND DISCUSSION

The computed temperature profiles are displayed in Fig. 2a, b. From the temperature profile, we can figure out the non-equilibrium steady state temperature within the dimer chains. In the present work, the materials in contact with the hot and cold heat baths are of the same type, A type in ABAB...ABA dimer chain or B type in BABA...BAB dimer chain. The temperature drop of the interfaces near the hot and cold heat baths is high compared to the temperature drop at interfaces away from heat baths. The phonon propagation from material B to material A is more resistive near the hot reservoir, while it is more resistive from material A to material B near the cold reservoir. This is due to high phonon scattering near the hot heat bath. The temperature jumps become smaller and smaller and thereby the temperature profile becomes linear as the mass of an oscillator of material B increases and approaches to the mass of an oscillator of material A. This happens

because of the decrease in mass mismatch of material A and material B at the interface.

The calculated values of temperature gradient and ITR at all the interfaces are shown in Fig. 3 and Fig. 4, respectively. The temperature gradient and ITR value are higher at the first interface near the hot reservoir in both dimer structures (i) and (ii) and are attributed due to higher phonon scattering rate near the hot heat bath. It is also seen that phonon flow is less thermal resistive while moving from a material of lower cut off frequency to a material of higher cut off frequency. In reversal case, phonon propagation from a material of higher cut off frequency to a material of lower cut off frequency is more thermal resistive. This happens in both types of dimer chains. As a result, the highest temperature gradient and ITR for ABAB...ABA dimer structure are observed at the second interface, while for BABA...BAB structure they are observed at the first interface.

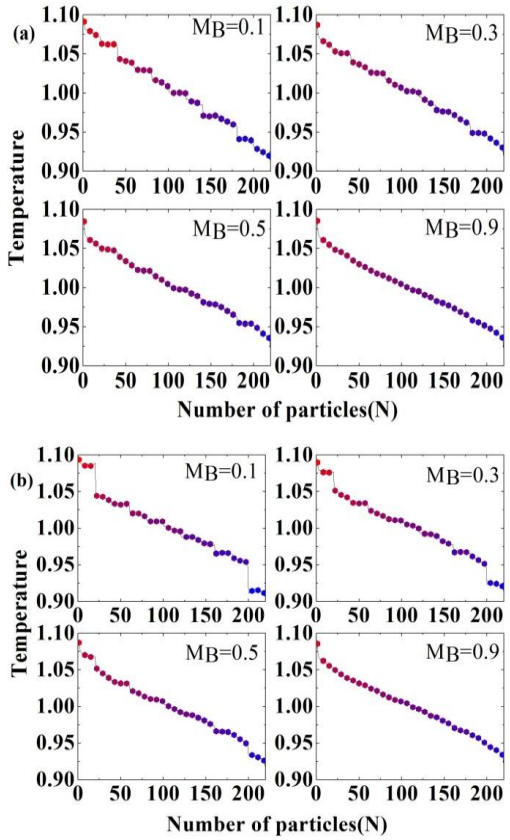


Fig. 2 – Temperature profiles of ABAB.....ABA dimer chains (a) and temperature profile of BABA.....BAB dimer chains

As we move from hot end to clod end, the temperature gradient at the interface gradually decreases. In the material structures we considered, the phonon frequency mismatch decreases as we go towards the cold end. Upon increasing the mass of an oscillator of material B, the temperature gradient and ITR decrease. It is seen that the temperature gradient and the ITR are high in BABA...BAB structure than those of ABAB...ABA structure.

The simulated results of heat flux and thermal conductivity are shown in Fig. 5 and Fig. 6, respectively. It is clearly seen that the heat flux and thermal conductivity of

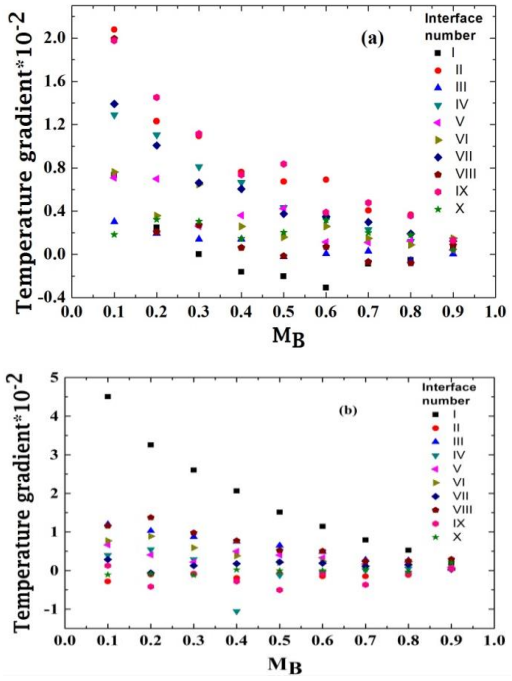


Fig. 3 – Temperature gradient at interfaces as function of the mass of an oscillator in B type segment: (a) ABABABABABA dimer chains, (b) BABABABABAB dimer chains

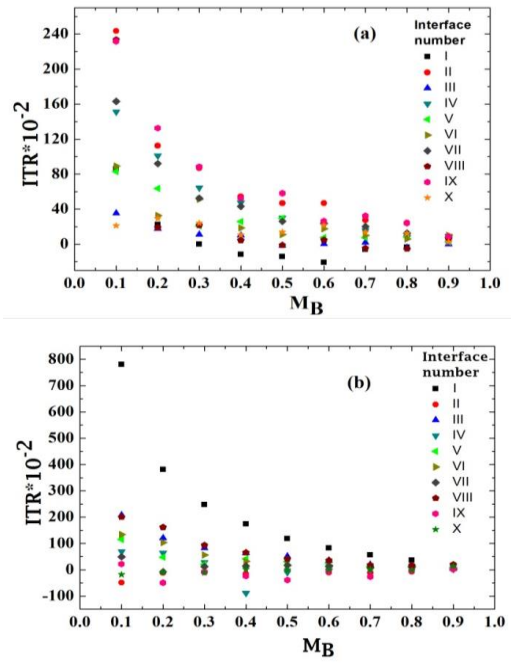


Fig. 4 – The ITR at interfaces as function of the mass of an oscillator in B type segment: (a) ABABABABABA dimer chains, (b) BABABABABAB dimer chains

these structures greatly depend on the mass mismatch of material A and material B. As the mass mismatch of materials A and B decreases, the heat flux and thermal conductivity increase. This increasein thermal conductivity is evidence of matching of phonon spectrum and density of states of the material constituents at the junction point of the interfaces. The heat flux and thermal conductivity of ABA….ABA dimer structure is higher compared to BAB….AB dimer structure. The phonon

attenuation is very high in structure BABA...BAB due to the lower mass of the material B connected with heat baths. Thus, the heat conduction in this multilayered dimer is also relying on selection of the material on the end points of the chain.

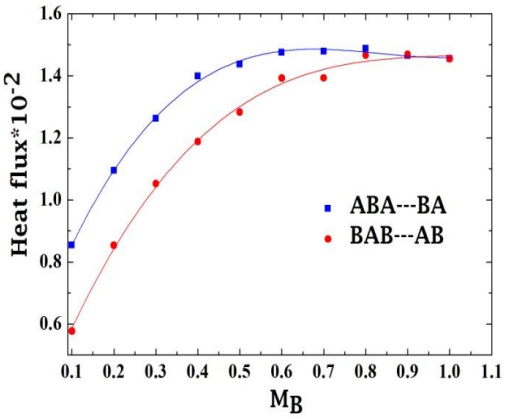


Fig. 5 – Heat flux of ABAB...ABA and BABA...BAB dimer structures

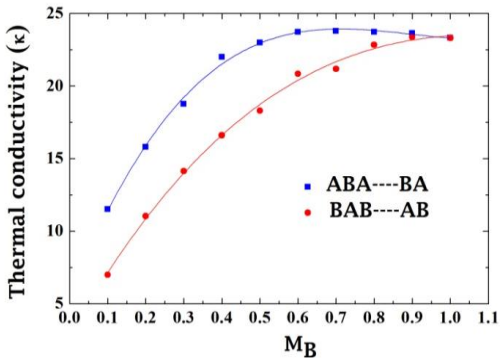


Fig. 6 – Thermal conductivity of ABAB...ABA and BABA...BAB dimer structures

4. CONCLUSIONS

In the present work, we studied the one dimensional multilayered dimer structure for its usefulness to control the phonon flow as a function of the mass mismatch. As the mass of the material of an oscillator in material B increases, the decrease in temperature gradient and ITR is noticed. The higher values of temperature gradient and ITR for ABAB...ABA structure are noticed at the second interface (B to A), while for BABA...BAB structure – at the first interface (B to A). The phonon transfer from material A to material B is less resistive than from material B to material A near the hot heat bath. We also conclude that the heat flux and thermal conductivity enhanced in both chains with increase in mass of material B. The decrease in mass mismatch in materials A and B leads to increase in the matching in vibrational modes of phonons and hence reduces the phonon attenuation at the junction point. The temperature gradient and ITR are higher in BABA...BAB dimer structure than those for ABAB...BAB dimer structure. It causes the reduction in thermal conductivity of BABA...BAB structure. The present work suggests that the thermal conductivity of the dimer structure is tuned by selecting the appropriate material in multilayered dimer chain. Such dimers could be very useful to construct the good quality thermal barrier in low dimensional structures. They may be also employed as the thermal connectors in low scale systems.

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Перенесення тепла в одновимірному димерному ланцюгу

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Явище перенесення тепла через одновимірний димерний ланцюг є важливим для розвитку нового покоління дрібномасштабних теплових приладів. Теплопровідність в одновимірній дво-компонентній структурі (подібної до димеру) вивчається за допомогою моделювання нерівноважної молекулярної динаміки. У цьому дослідженні розглядаються такі димери як AB….BA та BA….AB. В структурі ми взяли усього 11 шарів, і кожен шар має 20 осциляторів. Загальна кількість осциляторів цілого ланцюга становить $N = 220$. Крайні кінці димерного ланцюга з'єднані з тепловою ванною Ланжевена, щоб підтримувати постійну температуру на обох кінцях. Потенціал FPU-β використовується для обчислення міжмолекулярного потенціалу з $\beta = 1$. Температурний профіль, тепловий потік і теплопровідність вивчаються як функції маси осцилятора M_B (0,1; 0,2 … 0,8; 0,9) у шарі B. Маса кожного осцилятора у шарі A зберігається постійною і рівною $M_A = 1.0$, де $M_B < M_A$. Градієнт температури та термічний опір на кожному інтерфейсі розраховуються для обох димерних структур. Збільшення маси осцилятора шару B призводить до збільшення теплового потоку та теплопровідності структур. Виявлено, що ABABABABABA є більш теплопровідною структурою, ніж структура BABABABABAB. Таким чином, димер ABABABABABA є кращим теплопровідником, тоді як димер BABABABABAB є кращим термоелектричним матеріалом.

Ключові слова: Теплопровідність, Термічний опір інтерфейсу, Димерний ланцюг, Термоелектричні матеріали.