




Letter

Optimized interfacial thermal coupling between two nonlinear systems

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Abstract

Interfacial thermal resistance (ITR, or Kapitza resistance) is the bottleneck that limits the further growth of density for integrated circuit. In this paper, we study the interfacial thermal coupling between two nonlinear systems by using a one-dimensional FPU- β heterojunction model through molecular dynamics simulation. It is found that the ITR first decreases rapidly and then increases slowly with the increase of interface coupling coefficient (ICC). When the nonlinearity is weak, the optimal ICC can be explained by self-consistent phonon theory and effective phonon theory. We also find a double scale behavior in heterojunctions. The study of optimal interfacial thermal coupling for two nonlinear systems has potential applications in reducing the ITR between real materials.

Keywords: interfacial thermal resistance, molecular dynamics simulation, thermal properties

(Some figures may appear in colour only in the online journal)

Due to the rapid increase in power density of integrated circuit, poor heat dissipation caused by interfacial thermal resistance (ITR, or Kapitza resistance) becomes the bottleneck that limits the further development of electronics and information technology [1, 2]. How to couple materials to achieve optimized thermal transport is an urgent matter of concern [3]. At the same time, some promising low-dimensional thermal devices [4–7] have been constructed recently based on thermal rectification effect [8, 9], where the interfacial thermal transport plays an important role. Therefore, a deep understanding of interfacial thermal transport is crucial for both improving the

performance of electronic devices and designing new thermal devices.

In order to understand the physical mechanism of phonon transport across interface, different models have been brought up [10, 11]. However, most models offer limited accuracy of ITR predictions in nanoscale. They neglect the details of bonding in interfaces, which plays an important role in interfacial phonon transport. It can hugely change the ITR [3, 12–14] and has been demonstrated by different researches based on simulation and experiment [15–26]. Therefore, it is still urgent to understand the dependence of ITR on interfacial coupling and get the optimal ITR between two different systems.

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One-dimensional (1D) atomic chain has been widely used to research interfacial thermal transport [27–34], which provides general rules working in real materials. When coupling different 1D atomic chains, different interfacial coupling coefficient (ICC) makes great difference in interfacial thermal transport. For interfacial coupling between harmonic models, it is found that homogeneous chains have been proved to be the best thermal conductors [35]. For heterogeneous chains of harmonic model, the ITR reaches minimum when the coefficient of the coupling spring is the harmonic average of the linear coefficients of two chains [13]. However, how to obtain the optimized ITR between two nonlinear systems is still not clear.

In this work, we study the ITR of FPU nonlinear heterojunction model under different conditions. At first, the configuration and general form of the FPU heterojunction model are introduced. Then, the dependence of ITR on ICC is investigated through molecular dynamics (MD) simulation and the behind mechanism is discussed. Moreover, how the optimal ICC will vary with different parameters of FPU- β model is also investigated. The tendency fits the effective linear coefficient (ELC) deduced from self-consistent phonon theory (SCPT) and effective phonon theory (EPT).

For a general 1D lattice model, the Hamiltonian equation is shown as follows:

$$H = \sum_i H_i, \quad H_i = \frac{p_i^2}{2m_i} + V(x_{i-1}, x_i) + U(x_i). \quad (1)$$

Here the lattice is regarded as particle with a mass of m_i , and we only consider the interactions between the nearest neighbours. p_i is the momentum of the i th particle, x_i is the relative position of i th particle, $V(x_{i-1}, x_i)$ is the interaction potential between two adjacent particles, and $U(x_i)$ is the on-site potential from the external field.

The FPU heterojunction model considered in this work is shown in figure 1(a). The two FPU- β chains are connected by a spring with an elastic coefficient of k_{12} . The total model consists of 100 atoms. k_1, β_1 and k_2, β_2 are the linear and nonlinear coefficients of two FPU- β chains. The total Hamiltonian of the system can be written as:

$$H = H_{\text{FPU1}} + H_{\text{FPU2}} + \frac{1}{2} k_{12} (x_{i-1} - x_i)^2. \quad (2)$$

Where the Hamiltonian of the FPU parts are:

$$H_{\text{FPU}n} = \sum H_i, \quad H_i = \frac{p_i^2}{2m} + \frac{k_n}{2} (x_{i-1} - x_i)^2 + \frac{\beta_n}{4} (x_{i-1} - x_i)^4. \quad (3)$$

Throughout this paper, all quantities are unitless. x_i and p_i are the relative position and momentum of each atom. The temperature of each particle can be expressed as $T_i = \langle \dot{p}_i^2 \rangle$, and the heat flow of each particle can be expressed as $J_i = \dot{x}_i \cdot f_i$, where $f_i = -\partial V(x_{i-1}, x_i) / \partial x_i$ is the force applying on the particle [8], here $V = \frac{k}{2} (x_{i-1} - x_i)^2 + \frac{\beta}{4} (x_{i-1} - x_i)^4$. The equations of motions are determined and integrated by the Verlet-velocity method [36, 37], the thermal resistance can be expressed as: $R_i = (T_i - T_{i+1}) / J$ [38]. In order to establish

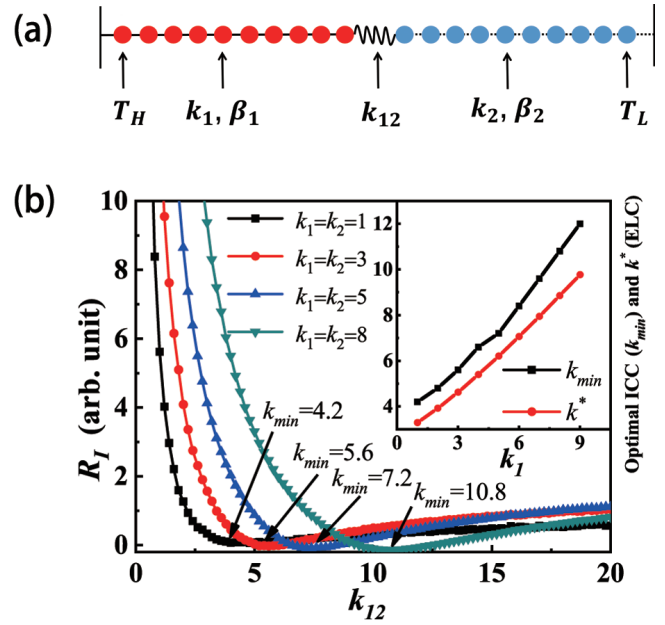


Figure 1. (a) Configuration of FPU- β heterojunction model. (b) ITR (R_I) versus ICC (k_{12}) as linear coefficient k varies and all $\beta_1 = \beta_2 = 1$. The inset is the optimal ICC (k_{min}) and the ELC(k^*) versus the linear coefficient (k_1) in the FPU- β model.

a temperature gradient, the system is coupled with Langevin thermostats [39] at the 1st and 100th atom with different temperature T_H and T_L , respectively. A finite temperature difference with 20% deviation from the average temperature was used. We thermalize the system with fixed boundary along the chain direction for 10^9 timesteps to guarantee it reaches steady state.

Our model considers phonon-phonon anharmonic process in chains. The widely used acoustic mismatch model (AMM) [11], diffusive mismatch model (DMM) [11] and atomic Green's function (AGF, or non-equilibrium Green's function) method [40] can only deal with harmonic process. So these models cannot deal with anharmonic system. However, different researches have shown that the anharmonic process plays an important role in interfacial phonon transport [11, 23, 41]. This is the advantage of our model.

Figure 1(b) shows the ITR (R_I) as the function of ICC (k_{12}) for different linear coefficients (k_1). With the increase of ICC (k_{12}), the ITR first decreases rapidly, then increases slowly. For weak coupling ($k_{12} < k_{min}$), the ICC gradually matches the spring coefficients of two chains when ICC increases. On one hand, the transport window for phonons to effectively transport is expanded. More phonons of higher frequencies can participate in transport. On the other hand, the decreases of mismatch between ICC and spring coefficients of two chains reduces interfacial phonon scattering. (Details explained later and shown in figure 2) When the ITR reaches the minimum point, the transport window opens to the maximum. After that, the mismatch between the ICC and two chains generates a greater impact on phonon transport. Thus, the increase of ICC no longer enables more phonons to participate in heat transport, but on the contrary, induces extra interfacial phonon scattering. This reduces the number of transmitted phonons and

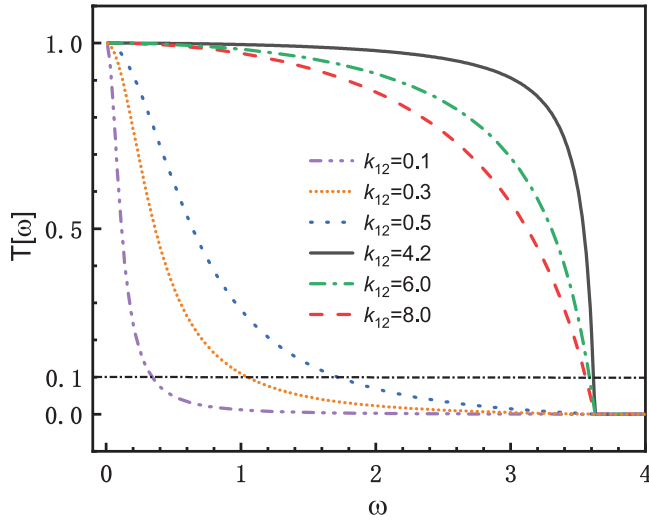


Figure 2. The frequency-dependent phonon transmission coefficient for different ICC in the one-dimensional FPU- β heterojunction model.

eventually increases the ITR. The inset shows that the optimal ICC with the minimum ITR, increases monotonically with the linear coefficient (k_1). What is more, the difference of ITR for cases with different k is small. This is because ITR is mainly affected by the interfacial phonon scattering induced by mismatch between ICC and spring coefficients of two chains after the minimum point. When ICC gets bigger, the difference of mismatch among different cases becomes smaller.

For homogeneous harmonic model, Zhang *et al* [13] reported that the minimum ITR occurs when the ICC equals to the spring coefficients of the atomic chains. On that account, in order to quantitatively show the above physical picture and further understand the relationship between ICC and k_1 , we calculate the effective linear coefficient (ELC) of FPU- chain, which is corresponding to the spring coefficients of harmonic model. The ELC is deduced from SCPT [32] and EPT [42].

We transform the Hamiltonian of the FPU- β model into the trial form of a harmonic model, that is

$$H_i = \frac{p_i^2}{2} + \frac{k^*}{2} (x_{i-1} - x_i)^2. \quad (4)$$

From SCPT, we have the optimal pseudophonon frequency:

$$\omega_p^2 = \frac{2}{m} \left[4\sin^2 \left(\frac{p\pi}{N} \right) \frac{\partial V}{\partial \gamma^2} \right]. \quad (5)$$

And two-point correlation function (in the classical form):

$$\gamma^2 \equiv \langle (x_{i-1} - x_i)^2 \rangle = \frac{k_B}{Nm} \sum_p \frac{4\sin^2 \left(\frac{p\pi}{N} \right)}{\omega_p^2}. \quad (6)$$

For FPU- β model,

$$V = \frac{k}{2} (x_i - x_{i-1})^2 + \frac{\beta}{4} (x_i - x_{i-1})^4. \quad (7)$$

Solving equation (5) self-consistently with equation (6), we can get the effective linear coefficient:

$$k^* = \frac{k + \sqrt{k^2 + 12\beta k_B T}}{2} \quad (8)$$

k_B is the Boltzmann constant. The details and thorough derivation of this expression is given by He *et al* in the appendix of [32].

To gain further insight into the dependents of ITR on ICC, we calculate the phonon transmission coefficient through AGF method [40, 43] for different ICC. (Corresponding to the case of black square in figure 1(a).) As the AGF method considers only harmonic process [7], we use the above ELC calculated by equation (8) during the calculation, which takes the nonlinear coefficients of two FPU- β chains into account. As shown in figure 2, the largest phonon transmission coefficients occur when the ICC equals to 4.2. The results are in accordance to the MD calculation. On one hand, when the ICC increases from 0.1 to 4.2, the transmission coefficients gradually decrease. Especially, the transmission coefficient first sharply decreases when the phonon frequency increases. This means that high frequency phonons are heavily blocked. Such that, the frequency range in which phonons can transmit across the interface increases as ICC increases, which is corresponding to the expanding of the transport window. This is because the ICC acts as the bridge to transport phonons from one chain to the other chain. According to lattice dynamics, phonon frequency is in proportion to the spring constant. When the ICC is 0, no phonon can transport across the interface. As the ICC gradually increases, phonons with higher frequencies can participate in transport.

To better clarify this point, we define a parameter, transmission window width (TWW), as the frequency range in which the transmission coefficient is larger than 0.1. When the ICC increases from 0.1 to 0.5, the TWW increases from 0.33 to 1.71. When the ICC equals to 4.2, phonons that contribute to heat transport cover the whole frequency range and the transport window opens to the maximum. What is more, the transmission coefficient for phonons within the transport window increases when the ICC increases from 0.1 to 0.5. Here, the ICC has only linear part. Phonons can only transport through harmonic process where two phonons have the same frequency. The mismatch of the ICC and spring coefficients of two chains will decrease the possibility that two phonons have the same frequency. Thus, less phonons will transport across the interface, and more phonons will be scattered [13, 17]. As a result, the decrease of mismatch between ICC and the spring coefficients of two chains decreases the interfacial phonon scattering.

On the other hand, when the ICC increases from 4.2 to 8.0, the transmission coefficients gradually decrease. This is corresponding to the increase of ITR in MD simulation. It should be noticed that, as the frequency increases, the transmission coefficient first decreases slowly, and then sharply decreases only in the high frequency ranges. This implies that the TWW keeps almost the same. The decreases in transmission coefficients come from the interfacial phonon scattering induced

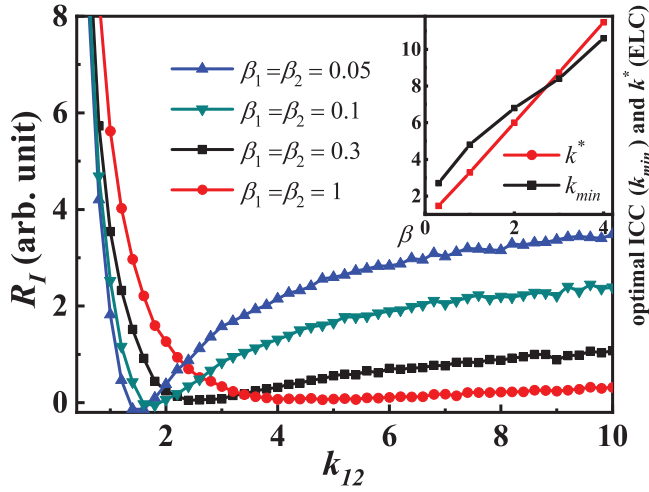


Figure 3. ITR (R_I) versus ICC (k_{12}) nonlinear coefficient β varies in homojunctions where all $k_1 = k_2 = 1$. The inset shows the optimal ICC (k_{\min}) and the ELC (k^*) versus the nonlinear coefficient β in the FPU- β model.

by the mismatch between the ICC and spring coefficients of two chains.

When the nonlinear coefficients of two chains increase from 0.05 to 1 (shown in figure 3), the ITR first decreases rapidly and then slowly increases as well. Although some of such high nonlinear coefficients cannot be realized in real materials nowadays, the change of nonlinearity is to explore the effect of nonlinearity on interfacial coupling. External fields, such as temperature [44] and strain [45], can modulate the nonlinearity of materials. Moreover, it is found that the ELC (k^*) and optimal ICC (k_{\min}) have the same trend in weak nonlinearity. It means that the ELC has a linear relationship with the optimal ICC when the nonlinear coefficient changes, which is in accordance to the rule in harmonic system [13]. Therefore, the optimal interfacial thermal coupling can be well explained by the ELC. So that, the ELC well demonstrate the relationship between the optimal ICC and the nonlinear coefficient. However, as shown in equation (8), obviously, the ELC is temperature dependent, which is different from the fact that nonlinear coefficient is independent of temperature. This is because the ELC is derived by keeping the thermal average in the canonical ensemble the same and viewing nonlinearity as part of the increase of linear coefficient [7, 32]. So the ELC is not the exact parameter in which the nonlinear effect is fully considered. As a result, the k^* and k_{12} shows some difference in absolute values.

It is also noticed that the ITR increases slower as the ICC increases when chains have a higher nonlinearity. This results in the larger differences of ITR for cases with different nonlinear coefficients compared with figure 1(b). This is because here the ITR is affected by both interfacial phonon scattering and phonon scattering in chains. When the nonlinear coefficients increase, the anharmonicity increases. The increase of anharmonicity will result in stronger phonon-phonon scattering, this point has been demonstrated in previous researches [46]. When phonons transport across the interface, they will experience stronger phonon scattering. Thus, these phonons

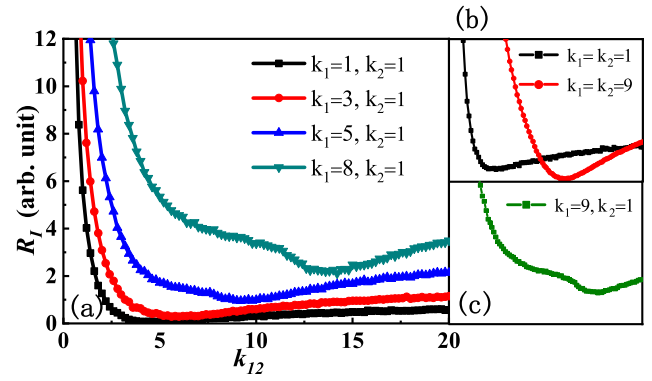


Figure 4. (a) ITR (R_I) versus ICC (k_{12}) as linear coefficient k varies in heterojunctions where all $\beta_1 = \beta_2 = 1$. (b) ITR (R_I) versus ICC (k_{12}) ($k_1 = k_2 = 1, 9$, $\beta_1 = \beta_2 = 1$). (c) ITR (R_I) versus ICC (k_{12}) ($k_1 = 9, k_2 = 1, \beta_1 = \beta_2 = 1$).

have lower possibility to be reflected back [47], and result in a lower ITR. So for cases with bigger nonlinear coefficients, the ITR will increase slower.

Figure 4 shows the relationship between ITR (R_I) and ICC (k_{12}) under different linear coefficients of the left chain. When the linear coefficient of the left chain increases, the minimum value of ITR also increases. This shows that the enhancement of interfacial mismatch increases ITR and enhances interfacial phonon scattering. When the linear coefficient of the left FPU chain keeps the same and the nonlinearity changes, we can also find that the ITR first decreases and then increases as the ICC increases. For weak nonlinearity, the optimal ICC increases with the nonlinearity of the left chain increases. Similarly, with the increase of nonlinearity, the phonon-phonon scattering effect is enhanced, and the influence of interfacial scattering on the ITR gradually decreases, so the rising trend of the ITR gradually slows down.

Another interesting phenomenon is the ITR shows a double scale behavior (shown in figure 4(a)). As the ICC increases, the ITR decreases fast at first, after reaching a certain point, decreases slowly. This two-stage decrease tendency becomes obvious when the gap between k_1 and k_2 increases (As shown in figures 4(b) and (c)). It can be understood from the superposition effect from two optimized interfacial thermal transport of linear coupling of nonlinear homojunctions. At the first stage, when the ICC increases from 0, the ICC gradually matches the spring coefficients of both chains. This is a superposition of two positive effects. Thus, the ITR decreases fast. However, as the spring coefficients of two chains has big difference, when the ICC increases to certain value, the further increases of ICC will increase the mismatch with the smaller spring coefficient, but decreases the mismatch with the larger spring coefficient. Thus, the second stage is a superposition of a positive and a negative effect. Thus, the ITR decreases slowly.

As shown in figure 5(a), when the nonlinearity of right chain equals to 1 ($\beta_2 = 1$), the minimum value of ITR decreases as β_1 increases, while in figure 5(b), when $\beta_2 = 0.1$, the minimum value of ITR increases. When β_2 is fixed to 1, the left chain tends to match the right chain and reduces the ITR. However, when β_2 is fixed to 0.1, the increase of nonlinearity of left leads them to mismatch and increases the ITR.

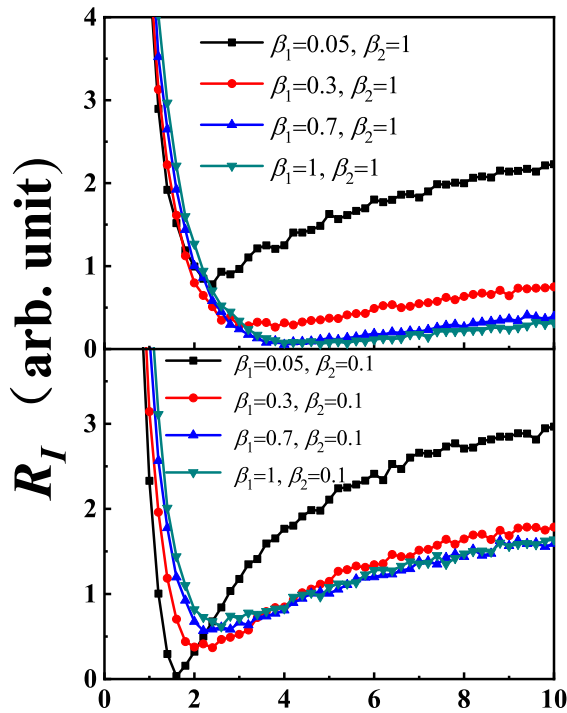


Figure 5. ITR (R_I) versus ICC (k_{12}) Here, all $k_1 = k_2 = 1$, (a) β_1 varies in heterojunctions as $\beta_2 = 1$, (b) β_1 varies in heterojunctions as $\beta_2 = 0.1$.

The results suggest that the ITR will reach the minimum when two nonlinear systems converge to a homogeneous system. In 2011, Zhang *et al* reported that the ITR reaches minimum when the coefficient of the coupling spring is the harmonic average of the linear coefficients of two chains in harmonic system [13]. In our anharmonic model, it is found that the simulation results agree with the principle of harmonic average only when the nonlinear coefficient is small. When the nonlinear coefficient becomes larger, the value of optimal ICC is larger than the theoretical value calculated from harmonic averaging and tends to diverge. By changing the coefficients of the right chain, we get similar results.

In summary, we have studied the ITR between two nonlinear one-dimensional models. It is found that as a general phenomenon in our model, with the increase of the ICC, the ITR first decreases rapidly and reaches a minimum point, then increases slowly. Moreover, it is found that the optimal ICC will vary with different coefficients of both chains. It fits the effective linear coefficient (ELC) deduced from the SCPT and EPT. We also find a double scale behavior of the ITR in heterojunction model as the ICC increases. This can be understood from superposition effect of two homojunctions. This work provides a theoretical reference for thermal transport across two nonlinear systems, which can inspire future manipulation of ITR between real materials.

As a final remark, we notice that the variation of ITR with ICC follows a general trend. The analytical expression of the ICC dependent transmission function for the harmonic system is derived in our previous work [13]. A possible extension of our work would be analytically derive a compact expression

for the general trend of the anharmonic system, which will gain further insight into the understanding of interfacial thermal coupling.

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