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Numerical simulation of heat transfer at the interface of dissimilar materials

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Abstract

Purpose – The small dimensions of future device designs also imply a stronger effect of material boundary resistance. For nanoscale devices and structures, especially, interface phenomena often dominate their overall thermal behavior. The purpose of this paper is to propose molecular dynamics (MD) simulations to investigate the mechanical and thermal properties at Cu-Al interface.

Design/methodology/approach – The two-temperature model (TTM)-MD model is used to describe the electron-phonon scattering at interface of different metals. Before the simulation of heat transfer process, a non-ideal Cu-Al interface is constructed by simulating diffusion bonding.

Findings – According to the simulation results, in unsteady state, the temperature distribution and the displacements of atoms near the interface tend to generate stress and voids. It reveals the damage mechanics at the interface in heat transfer.

Originality/value – The atomic model proposed in this paper is computationally efficient for interfacial heat transfer problems, and could be used for investigation of other interfacial behaviors of dissimilar materials.

Keywords Metals, Heat transfer, Thermal resistance, Diffusion, Bonding, Temperature distribution
Paper type Research paper

Nomenclature

E	potential energy of the system	N	number of atoms
$F_i(\rho_i)$	embedding energy of atom i with electron density ρ_i	v_i	velocity of atom i
q	heat flux	r_{ij}	separation distance between atoms i and j
h	heat transfer coefficient	f_{ij}	interactive force between atoms i and j
kB	Boltzmann constant	$F_{ij\alpha}$	the α-component of the force exerted on atom i by atom j
m	mass		

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R_B	thermal boundary resistance
T	temperature
t	time
Γ	transmission coefficient of the material of origin for the mode of propagation
θ	angle of incidence
$\sigma_{\alpha\beta}$	internal stress
ρ_i	electron density
ρ	material density
$\varphi_{ij}(r_{ij})$	two-body central potential between atoms i and j, with the separation distance r_{ij}
Ω	volume
C	heat capacities
K	thermal conductivities
e	index to indicate electron
l	index to indicate lattice
G	the electron-phonon coupling factor
$\vec{F}_i$	the force acting on atoms i due to the interatomic potential
ξ	a coefficient that describes the coupling between the electrons and lattice
G_b	the bulk electron-phonon coupling factor

1. Introduction

Heat transfer across interfaces is a critical consideration in a wide variety of scientific and engineering applications. This is especially true for nanoscale devices and structures, where interface phenomena often dominate their overall thermal behavior (Sungtaek Ju, 2005). Hence, it is essential to understand the effect of material parameters on the interfacial mechanisms of dissimilar materials under thermal flux conditions. However, the determination of the stress and strain fields in multi-layers system presents difficulties arising from the step-wise geometry and dissimilar material properties. Although finite element models include the complexities arising from the geometry and dissimilar materials, they fail to accurately capture the singular stress field at the sharp corners and cracks, resorting to sub-modeling (Kay *et al.*, 2006). Few estimates exist on the magnitude of the thermal boundary resistance between dissimilar materials. As more materials are introduced in semiconductor processing, there is a growing need to understand the magnitude of boundary thermal resistance and its significance in future nanoscale device behavior (Pop and Goodson, 2006). When the system becomes extremely small, the atomistic effects have to be taken into account correctly. At the nanoscopic length scale the molecular dynamics (MD) method takes correctly into account these effects, when the potential is chosen correctly.

The microstructures of Cu/Ta interface and SiO_2/Si interface were analyzed by MD simulations (Heino, 2001; Watanabe *et al.*, 2004), while the conditions applied were different from the actual processes of interface forming which involve high temperature and high pressure. To construct a non-ideal interface, high pressure and temperature conditions are applied to the system. Because temperature and pressure play important roles in interface forming. MD simulations results (Weissmann *et al.*, 1992) show that interfacial amorphization clearly develops at higher temperatures for Co-Zr interface. Volz *et al.* (2000) investigated the interfacial effects in silicon-germanium superlattices by MD and discovered that strain greatly affects the overall thermal conductivity of the superlattices, and showing an improved agreement with experimental values. Abramson *et al.* (2002) used NEMD simulations to study how various factors affect the thermal conductivity of bi-material thin films. Stevens *et al.* (2007) utilized NEMD to investigate thermal transport across solid-solid interfaces. One of the key findings of their study is that there is a significant interfacial thermal

transport dependence on temperature for the interfaces, it suggesting that inelastic scattering of phonons at the interface plays a major role in thermal transport.

In dielectric materials or semiconductors, the contribution of electron on thermal transport across the interface is negligible. However, electrons are the dominant thermal carriers for metals, and electron-phonon scattering at interface play an important role in transport mechanism for dissimilar materials (Stevens *et al.*, 2007). A two-temperature model (TTM)-MD model (Ivanov and Zhigilei, 2003) that combines the MD method for simulation of fast non-equilibrium processes with a continuum description of the electronic heat conduction is proposed to account for the electron scattering. The model is based on the TTM, which was originally developed for strong electron-phonon non-equilibrium due to the fast electronic excitation. Moreover, the TTM-MD model is also applicable for the description of the electronic heat conduction in a material undergoing shock wave heating (Ivanov and Zhigilei, 2003).

In this paper, MD simulations of heat transfer at Cu-Al interface are proposed. The TTM-MD model is used to describe the electron-phonon scattering at interface of different metals. To construct a non-ideal interface, a simulation of diffusion bonding for Cu and Al is added before the heat transfer simulation. Based on the proposed model, the thermal properties of Cu-Al interface are investigated.

2. Model construction

The embedded atom method (EAM) is used to describe the interatomic interactions between Al-Al, Cu-Cu, and Al-Cu. EAM defines the energy E of the system as the sum of energies for each atom i, with each atom having energy contributions from an embedding function F that depends on a local electron density and a pair potential, so that (Mei *et al.*, 1991)

$$E = \sum_i F_i(\rho_i) + \frac{1}{2}\sum_{i \neq j} \phi_{ij}(r_{ij}) \tag{1}$$

where $\phi_{ij}(r_{ij})$ is a two-body central potential between atoms i and j with the separation distance r_{ij} and $F_i(\rho_i)$ is the embedding energy of atom i with the electron density ρ_i. The Velocity-Verlet algorithm (Swope *et al.*, 1982) was used to march the atoms through time. It is an extension to the standard Verlet method, which is accurate to the third order of the time step size. The instantaneous temperature of each site at a certain time step is taken as the mean temperature over a neighborhood of atoms enclosed by a sphere of a radius r (Li *et al.*, 2003). The heat flux through a volume is calculated as (Maruyama, 2000)

$$q = \frac{1}{2V}\left[\sum_i^N m_i v_i^2 v_i + \sum_i^N \sum_{j \neq i}^N \phi_{ij} v_i - \sum_i^N \sum_{j \neq i}^N (r_{ij} f_{ij}) v_i\right] \tag{2}$$

where the first and second terms related to summations of kinetic and potential energy carried by a molecule *i*.

In this MD model, the expression of the thermal boundary resistance is given as (Hegedus and Abramson, 2006)

$$R_B = [\frac{\pi^2}{15}\frac{k_B^4}{h^3}\left(\sum_j v_{1,j}^2 \Gamma_{1,j}\right)^{-1} T^{-3} \tag{3}$$

where T is the temperature at the interface, and Γ is the transmission coefficient of the material of origin for mode of propagation j, which is defined as

$$\Gamma_{1,j} = \int_{\theta=0}^{\pi/2} \alpha(\theta)_{1\to 2} \cos(\theta)\sin(\theta) d\theta \tag{4}$$

where θ is the angle of incidence.

The internal stress is given by virial stress (Fabrizio, 2001)

$$\sigma_{\alpha\beta} = \frac{1}{\Omega}\left(\sum_i m_i v_{i\alpha} v_{i\beta} + \frac{1}{2}\sum_{i\neq j} r_{ij\beta} F_{ij\alpha}\right) \tag{5}$$

where α, β = x, y, z denote Cartesian components and the sums extend over all the atoms in a selected box of total volume Ω, $v_{i\alpha}$ is the α-component of the velocity of atom i, $r_{ij\beta}$ is the β-component of the vector r_{ij} separating atoms i and j, and $F_{ij\alpha}$ is the α-component of the force exerted on atom i by atom j.

The TTM-MD model is used to describe the electron-phonon scattering at interface of different metals. TTM describes the time evolution of the lattice and electron temperatures by two non-linear differential equations, the two equations coupled by a term responsible for the energy exchange due to the electron-phonon coupling:

$$C_e(T_e)\frac{\partial T_e}{\partial t} = \nabla[K_e(T_e)\nabla T_e] - G(T_e - T_l) + q^m \tag{6}$$

$$C_l(T_l)\frac{\partial T_l}{\partial t} = \nabla[K_l(T_l)\nabla T_l] + G(T_e - T_l) \tag{7}$$

In the TTM-MD model, the MD method completely substitutes the TTM equation for the lattice temperature. The electron system and the lattice system are modeled by a continuum model and an atomic model, respectively. The electron and lattice are coupled by adding a term to the force of atom, the corresponding equation is (Ivanov and Zhigilei, 2003)

$$m_i \frac{d^2 \vec{r_i}}{dt^2} = \vec{F_i} + \xi m_i \vec{v}_i \tag{8}$$

where

$$\xi = \frac{G_b V_N (T_e - T_{l,N})}{\sum_i m_i v_i^2} \tag{9}$$

where m_i and $\vec{r_i}$ are the mass and position of atom i. $\vec{F_i}$ is the force acting on atoms i due to the interatomic potential. ξ is a coefficient that describes the coupling between the

electrons and lattice within a discretized cell with a volume of V_N and lattice temperature of T_N. G_b is the bulk electron-phonon coupling factor, which describes the linear rate at which energy is transferred between the electron and lattices system per unit volume.

3. Simulations and analysis

3.1 Model construction

MD model initiated as the following: selecting Cu and Al as simulation materials, and formed as face-centered cubic (FCC) structure. The two dimensions are in x – [1 0 0] and z-[0 0 1]. The time step size used in each simulation was 1 fs. The cut off distance in all cases was $r_c = 2.5\sigma$, and σ is the (finite) distance at which the interparticle potential is zero. Periodic boundary conditions are implemented in x and y directions to simulate an infinite film in the direction. Three layers of boundary atoms on top and bottom were fixed. The five layers of atoms adjacent to fixed atoms were defined as cold bath and warm bath, respectively. The energy is added and removed through warm bath and cold bath at every time step, and a heat flux was induced in z direction. The distance between Cu block and Al block is initialized as the average of characteristic length scale for Cu and Al. The model was initialized as shown in Figure 1.

To construct a non-ideal Cu-Al interface, the system is equilibrated at 300 K at first for 10,000 time steps, and then is heated to 800 K, the increase rate of temperature is 6×10^{13} K/s. At the same time, the external pressure is applied to vertical direction, which is 15 MPa. To obtain sufficient interaction between atoms of different materials at interface, the temperature of system is kept at 800 K for 200,000 time steps. And the sample was quenched (down to 300 K) for 100,000 time steps, which will lead to the formation of a disordered layer at the interface. Then the quenched structures are the relaxed by allowing all atoms to move and reach the minimum energy configuration. Three layers of boundary atoms at top and bottom serve as purposes of load and displacement.

3.2 Simulation results

3.2.1 The properties of the constructed interface. The region where the concentration of the solute atoms is over 5 percent is defined as the interfacial region. As shown in Figure 2, at 500 K, the thickness of interfacial region increases firstly, and after about 9,000 time steps then the thickness reaches about 0.7 nm and does not show further increase except for minor fluctuations. The profile for 650 K is similar to that for 500 K, except that the maximum thickness value is higher. While at 800 K, the thickness increases rapidly and continuously without saturation over the duration of the calculation; and a significant change of interfacial thickness can be observed at 7,000 time steps, which is earlier compared with the 500 K case and the 650 K case. In steady state, the thickness of interfacial region increases with the increase of temperature.

The displacements of the boundary atoms are controlled to generate tensile deformation. Each loading increment corresponds to a strain of 0.25 percent and is followed by a period of equilibration at constant strain. Based on the stress-strain curves as shown in Figure 3, for all the cases, after reaching the maximum stress, the stress drops precipitously and plastic flow occurs. The tensile strength of the constructed interface can reach 82 percent of that for the ideal-contact interface, demonstrating the effectiveness of diffusion-bonding process in creating bonds between the two materials. The interface models contain no initial defects, such as

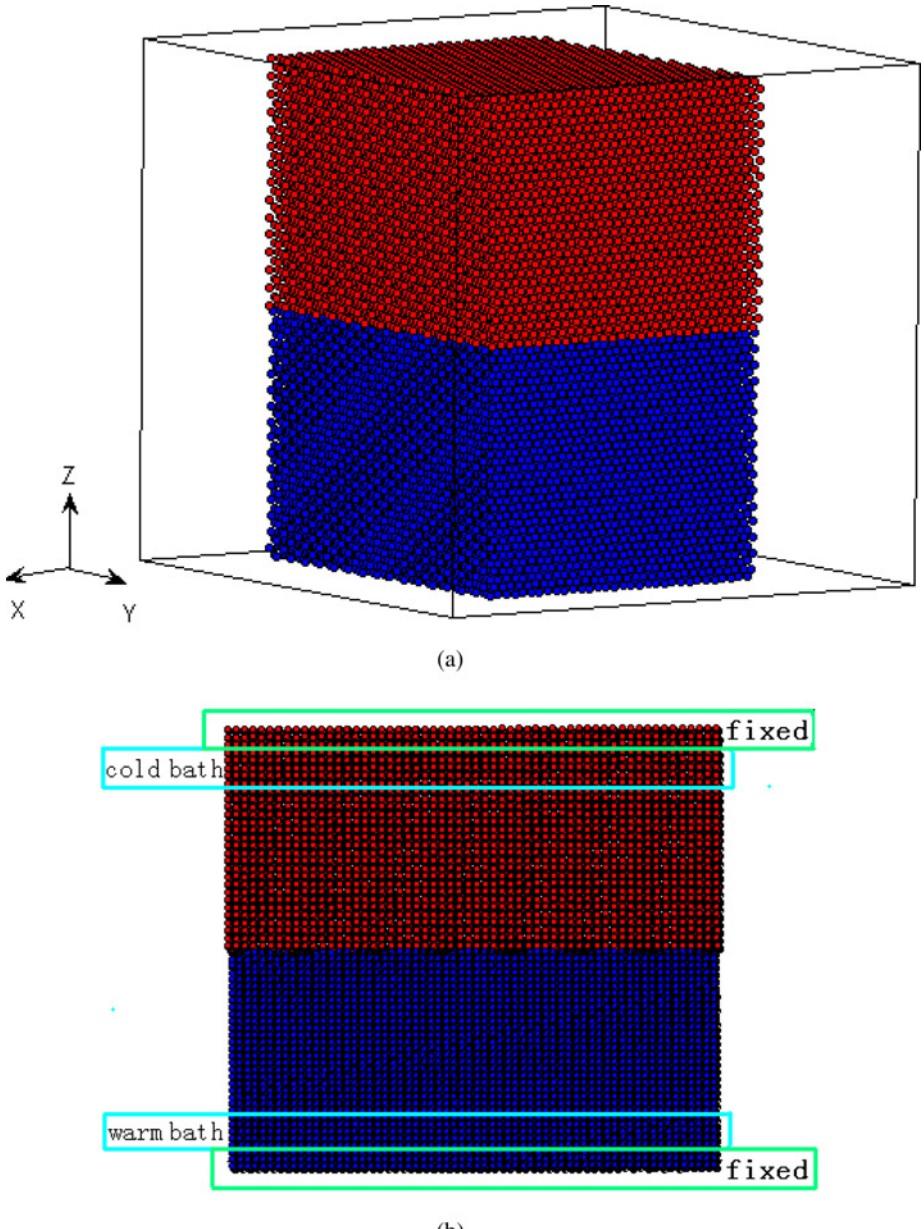


Figure 1.
Model configuration

Notes: (a) The initial model configuration and (b) the generation of thermal flux

voids and impurities, hence, the strength values here are higher than those from experiments.

3.2.2 Thermal properties in unsteady state. The temperatures of atoms layer in steady state were studied in Abramson *et al.* (2002) and Stevens *et al.* (2007), while very

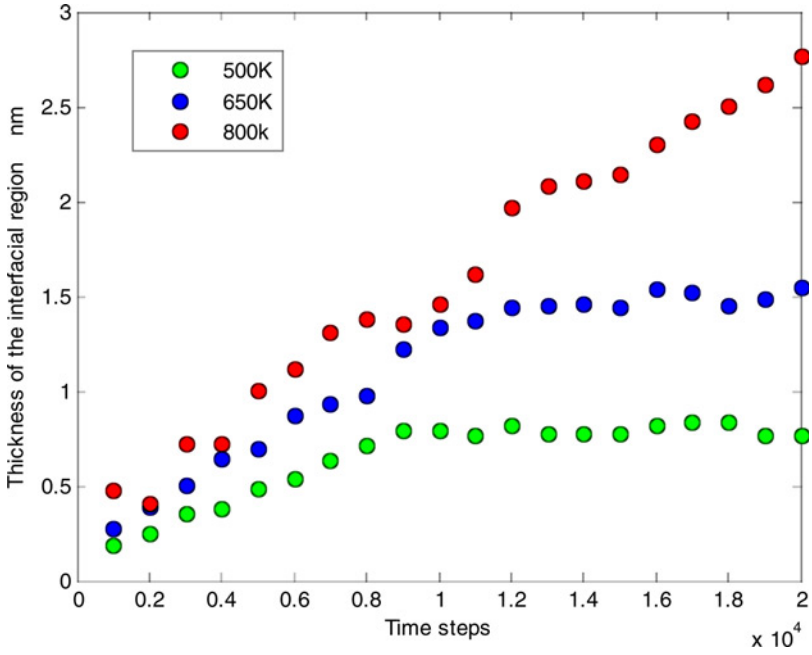


Figure 2.
Thickness of interfacial region at different heat source temperature

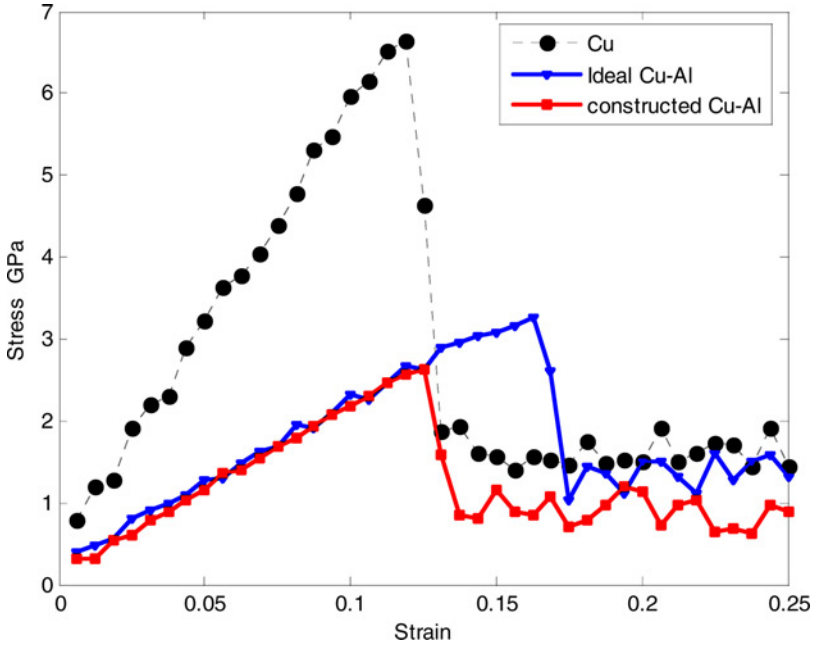
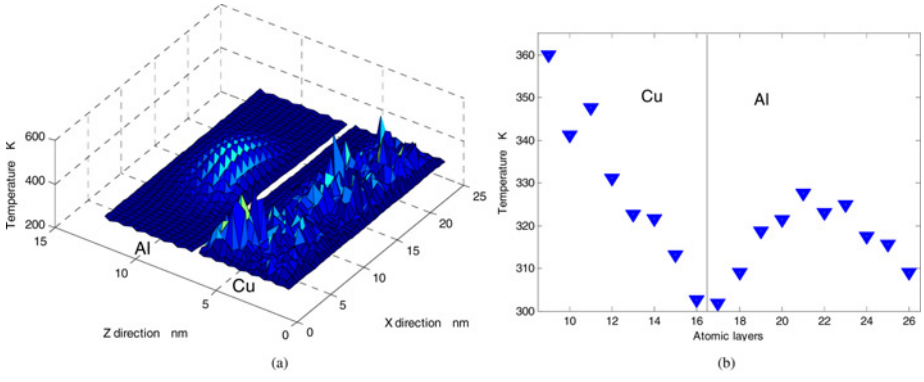


Figure 3.
Stress-strain curves of different models

few results of temperature distribution along the interface and in unsteady state are presented. The results in unsteady state are analyzed here, which may be useful to understand the interfacial mechanisms. Before a steady state is reached, at 12,000 time steps, the temperature distribution near the interface is shown in Figures 4(a) and (b) presents the average temperatures of the atomic layers. It is known that the temperature will drop suddenly at the interface owing to the interface thermal resistance. For our simulation results, the interesting point that is to be noted is that right at the interface there is a jump in temperature, the temperature near the interface decreases at first and then increases severely. Since the temperature distribution is not uniform along the interface, as shown in Figure 4(a), the thermal fluxes are different along the interface in unsteady state, which will cause high temperature region formed in Al block. It also means large temperature difference exists at the interface, which will generate stress and cracks eventually.

The heat transfer across the dissimilar materials interface takes place through surface-asperity micro-contacts and through air-filled micro-gaps, and is, hence, associated with a significant thermal resistance. However, there is very few studies focus on how interatomic interaction at interface effect on the thermal resistance, while it can be easily researched here. As shown in Figure 5, for smooth interface, the thermal resistance can also be generated by interatomic interaction. In primary stage, the interfacial thermal resistance is unstable and will become very large at certain time. At the last stage, the change of interfacial thermal resistance tends to be stable. The variation of interfacial thermal resistance with time is quite similar to the experimental results obtained by Masse (Massé *et al.*, 2004).

The vector field results of atoms displacements are shown in Figure 6. The Cu atoms move with opposite direction to Al atoms along the interface, as shown in Figure 6(a). The similar results on the displacement of different sides were observed in interfacial fracture experiments for dissimilar materials in electronic packages (Kay *et al.*, 2006). The movements will generate voids and internal stress, which may give an explanation for the crack generation mechanics at interface of dissimilar materials. To prove the explanation, two blocks of Cu are chosen to build up the interfacial model. For the Cu-Cu interface, as shown in Figure 6(b), the atoms of different blocks tend to move toward interface, but there is almost no movement along the interface (x direction), which is different with the atoms shown in Figure 6(a). By the



Notes: (a) The temperature distribution near the interface and (b) average temperatures of the atomic layers near the interface

Figure 4.
Temperature distribution at 12,000 time steps

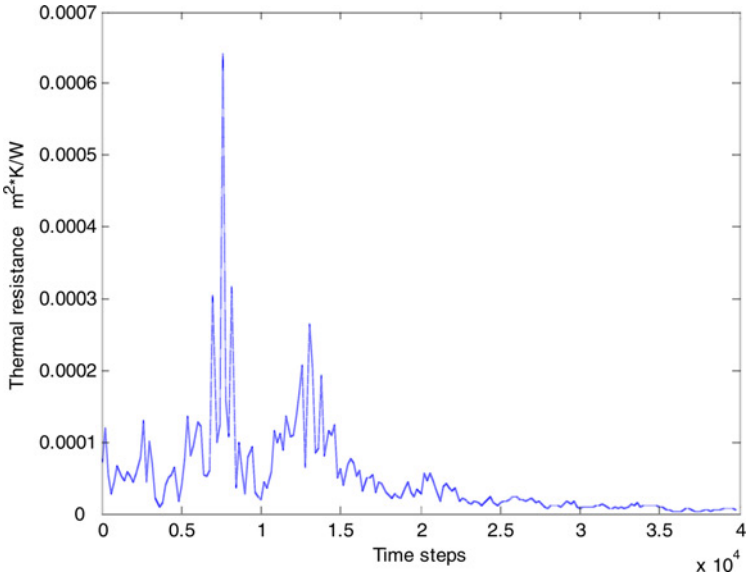


Figure 5.
Time dependent of interfacial thermal resistance

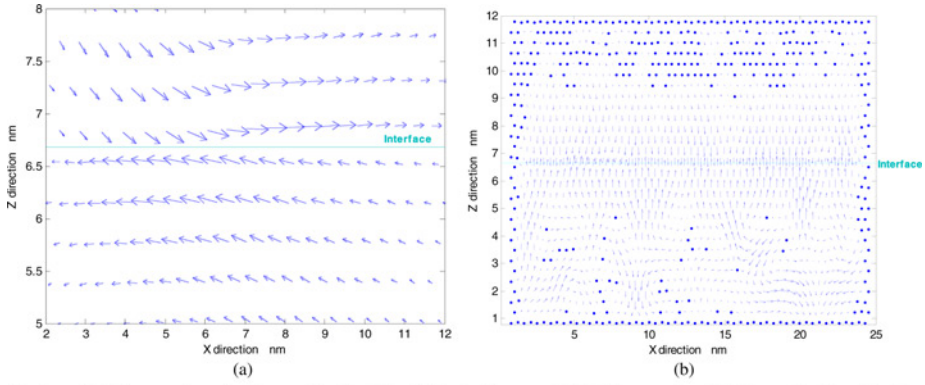


Figure 6.
Vector field results of atoms displacements near the interface at 20,000 time steps

Notes: (a) The vector field results for Cu-Al interface and (b) the vector field results for Cu-Cu interface

comparative study, it is concluded that the characteristic of atoms' moving along the interface is caused by dissimilarity of material, which reveal the damage mechanics at the interface in heat transfer.

3.2.3 The effects of electrons on heat transfer between metals. According to the simulation results, as shown in Figure 7, there is no big difference in thermal resistance for the Cu-Al interface by MD model and the combined model. According to the simulation results of Ivanov and Zhigilei (2003), comparing with the TTM model, a very similar temperature and pressure distributions are observed in MD simulations without the electron heat conduction, the effect of the electronic heat conduction is relatively small for metal-metal interface. While the difference of the thermal resistance calculated by the two models tend to be larger when the heat source temperature

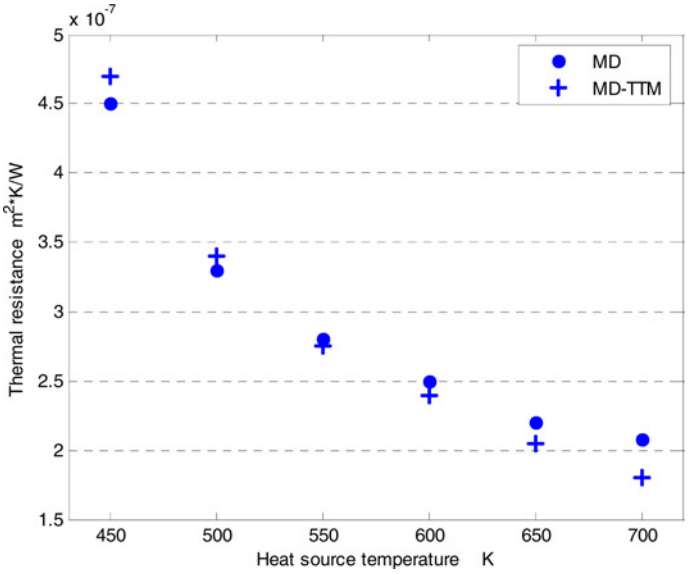


Figure 7.
Thermal resistances calculated by MD model and TTM-MD model

increase, as shown in Figure 7. This may because the electron can play a significant role when the maximum local temperature reached is close to the melting point, in this case the electronic heat conduction may prevent melting in a system that would otherwise melt in a pure MD simulation (Ivanov and Zhigilei, 2003). On the other hand, for interfaces between a metal and dielectric material (Stevens *et al.*, 2007), it was found that poor electron-phonon coupling could result in a significant resistance, and the added resistance is negligible for highly mismatched interfaces and only needs to be considered for high quality interfaces.

4. Conclusion

In this paper, an atomic model is proposed to study the properties on interface of dissimilar materials in heat transfer. To obtain a more accurate model, the interface construction is implemented before the heat transfer simulation. The results show the tensile strength of the constructed interface can reach 82 percent of that for the ideal-contact interface, demonstrating the effectiveness of diffusion-bonding process in creating bonds between the two materials.

According to the simulation of heat transfer through Cu-Al interface, before a steady state is reached, the temperature distribution is non-uniform along the interface and several places corresponding to large temperature difference. Moreover, the atoms of dissimilar materials move with reverse direction along the interface. It will cause stress and voids near the interface, which will cause crack eventually. On the other side, for the Cu-Cu interface, there is almost no movement along the interface for the atoms of different blocks. It is concluded that the movements of atoms along the interface are caused by dissimilarity of material.

There is no big difference in thermal resistance for the Cu-Al interface by MD model and the combined model. While the difference in thermal resistance for the two models tend to be larger when the heat source temperature increases. This may be because the electron can play a significant role when the maximum local temperature reached is

close to the melting point, in this case the electronic heat conduction may prevent melting in a system that would otherwise melt in a pure MD simulation.

The proposed atomic model was computationally efficient for interfacial heat transfer problems, and it could be used as well as for investigation of other interfacial behaviors of dissimilar materials.

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