Molecular Dynamics Simulation of Heat Transfer at Contact Interface of Hot Forming Die

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Molecular Dynamics Simulation of Heat Transfer at Contact Interface of Hot Forming Die

Baoshan Lu[1], Leigang Wang[1] and Xiang Ma[2*]

[1] School of Materials Science and Engineering, Jiangsu University, Zhenjiang 212013, China
[2] SINTEF Industry, POB 124, Blindern, 0314 Oslo, Norway

xiang.ma@sintef.no

Abstract. During metal hot forming process, the billet and the die interact by contact under high temperature, high pressure and severe sliding. In this paper, an atomistic approach is utilized to study the behaviour of heat transfer at the contact interface of hot forming die and the material. Based on non-equilibrium molecular dynamics and phonon scattering theory, the phonon heat transfer process at the billet/die rough interface at nano-scale is analysed. The effects of interfacial lattice defect concentration and average interfacial temperature on the phonon heat transfer coefficient are examined. It is found that when the lattice defect concentration increases the phonon mismatch at the interface deteriorates and the interfacial thermal resistance increases, which leads to a sharp decrease in phonon heat transfer coefficient. A higher temperature of the contact body and a higher average interface temperature lead to a higher probability of inelastic scattering of phonons at the interface. Moreover, the high frequency phonons at high temperature might be decomposed into two or more low frequency phonons during the energy transmission, which increases the propagation of phonon at the interface; thus the phonon heat transfer coefficient increases accordingly.

1. Introduction

The influence of incompletely contacted interface on heat transfer is an important topic in the field of micro-scale heat transfer. Molecular dynamics (MD) calculation is an effective method to carry out research on this subject to estimate some thermophysical properties which are difficult to be obtained experimentally. However, there has been few public reports on the heat transfer at the solid metal contact interfaces. There are two main reasons for this: (1) there is a lack of potential functions to precisely describe the atomic interactions of alloyed materials or dissimilar interfaces; (2) the MD method mainly studies the heat conduction problem caused by phonons, while the heat conduction in solid metal is dominated by free electrons where the phonon heat conduction only accounts for a small proportion of the global thermal conductivity [1]. It is generally believed that this small proportion of phonon thermal conductivity do not reflect the overall characteristics of solid metal interfacial heat transfer. These have become the bottleneck restricting the application of MD to the study of solid metal interfacial heat transfer.

However, for metals with lower thermal conductivity such as Ni, the thermal conduction caused by phonons cannot be ignored, especially at the micro/nano scale interface where the free electrons are limited by the surface and size effect leading to a sharp decrease in heat conduction [2]. The same could be true for the billet/die interface in hot forming. The rough or imperfect contact interface of the billet/die carries various non-metallic inclusions such as air gap, nitride layer, oxide layer or oil stain.

These non-metallic inclusions greatly inhibit the free electron conduction, while the phonon heat conduction is significantly enhanced and rapidly becomes the dominant factor in heat transfer. Therefore, this paper will use a non-equilibrium Molecular Dynamics method (NEMD, [3]) to examine the phonon heat transfer behaviour in an asymmetric billet/die interfacial model. The effects of the interfacial lattice defect and the average interfacial temperature will be studied.

2. F-S potential function and the NEMD model

In the MD simulation, the selection of the interaction potential between the particles in the system is very important as it determines the precision of the simulation results and the computational time. One effective potential energy model for the metallic atomic system is the multi-body potential such as the Finnis and Sinclair model (F-S) which is based on the tight-binding theory of metallic energy bands [4]. The F-S potential function is chosen in this paper for the MD calculation of a heterogeneous Fe-Ni atomic system, close to the hot forming application where the main alloy elements are Fe (in a typical H13 steel die) and Ni (in a GH4169 superalloy billet). The F-S potential parameters of Fe and Ni is obtained from the literature [4].

The NEMD method requires a temperature gradient between the atomic layers of the thermally conductive region. The thermostat method is used to apply thermal disturbance to the heat conduction zone along the thickness or Z directions of the hot zone (the billet) and the cold zone (the die) respectively [3]. If the statistical heat flow in the system is J_z and the interfacial temperature difference is ΔT, then the interfacial heat transfer coefficient h_{ph} (or phonon heat transfer coefficient) caused by phonon action is give as:

$$h_{ph} = J_z / \Delta T \tag{1}$$

The relationship between the phonon heat transfer coefficient h_{ph} and the global interfacial heat transfer coefficient (IHTC) is that h_{ph} is the part of IHTC and accounts for a large proportion of IHTC values at the micro/nano-scale incomplete contact interface.

During the simulation, the atomic motion equation is numerically integrated using the velocity Verlet algorithm. The integration step is set to 4 fs and the total integration step is 3 million. The total simulation time t_s is 12 ns. Among them, the first 9ns is used for the initial balance of the system and the last 3ns is used to calculate the temperature of each atomic plane and the heat flow.

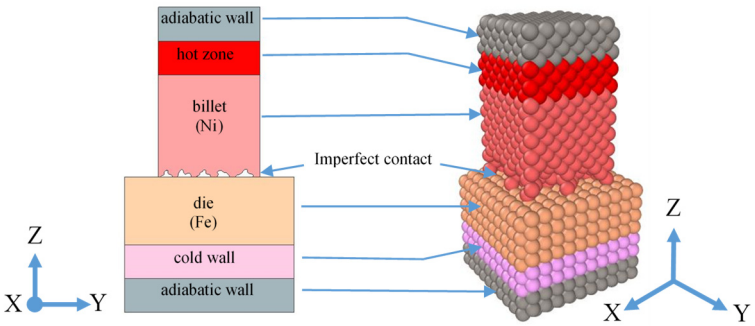


Figure 1. MD model of heat transfer at asymmetric interface

An asymmetric interfacial heat transfer MD model is constructed as shown in Figure 1, in which the periodic boundary conditions are applied in the X and Y directions. The superlattice composed of Ni atom (face-centered cubic structure) and Fe atom (body-centered cubic structure) forms an asymmetric contact interface, and the Ni atoms are randomly removed to indicate its incomplete contact with the surface of the Fe atoms. The cross-section (XY plane) of the model is square in which the Fe atomic layers are 10UC×10UC (UC is the unit cell) and the Ni atomic layers are 5UC×5UC. The thicknesses of the heat conduction zones of the Ni and Fe atomic layers are 6UC and 4UC, respectively. To prevent atoms on the surface of the hot and cold regions from escaping from the system, a layer of adiabatic wall with 2UC is added on the outer side of the hot and cold regions, respectively. The maximum temperature difference in the system is 100 K.

3. MD simulation results and discussions

3.1 Effect of interfacial lattice defect concentration on phonon heat transfer coefficient

A certain proportion of Ni atoms are randomly removed at the billet/die interface to simulate the effect of incomplete contact on the phonon heat transfer coefficient. The ratio of the number of Ni atoms deleted at the interface to the total number of Ni atoms in the heat transfer region indicates the interfacial lattice defect concentration. Figure 2 shows the temperature distribution along the Z direction when the pre-set temperatures of the hot and cold regions are 673 *K* and 573 *K*, respectively, and the interfacial lattice defect concentration of Ni is 5%. It can be clearly seen that the temperature in the vicinity of the hot and cold regions is nonlinear, while the temperature in the region far away from the hot and cold regions is approximately linear. The temperature in the heat conduction region of the Ni atom decreases rapidly. In the heat conduction zone of Fe atom, the heat resistance encountered is small when the heat flow flows through the Fe atomic layer, which is due to that the thermal conductivity of Fe atom is much higher than that of Ni atom. Thus, the temperature change in the Fe region is much smoother than in the Ni region. At the Ni/Fe contact interface, there is a significant temperature discontinuity due to the sudden lattice discontinuation, as high as 36.4 *K*.

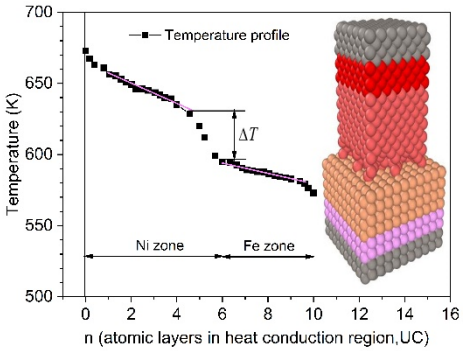


Figure 2. Temperature distribution of Ni/Fe atomic system.

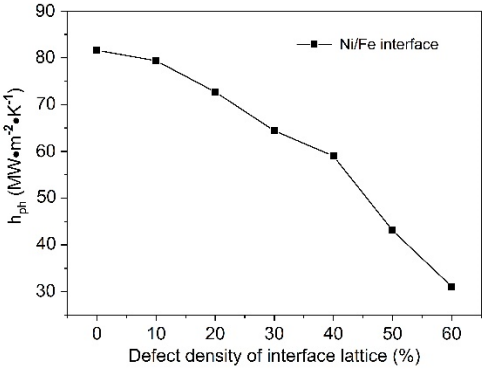


Figure 3. Variation of h_{ph} with defect density of interface lattice.

Figure 3 shows the relationship between h_{ph} and the interface lattice defect concentration when the preset temperatures of the hot and cold domains are 673 *K* and 573 *K*, respectively. As the interfacial lattice defect concentration increases, the interfacial thermal resistance increases and h_{ph} decreases accordingly. When the interfacial lattice defect concentration is less than 40%, h_{ph} decreases slowly with the increase in the interfacial lattice defect concentration. But when the defect concentration exceeds 40%, the phonon mismatch at the interface deteriorates, resulting in h_{ph} dropping rapidly.

To examine the effect of the phonon mismatch at the interface on the interfacial heat transfer, the density of phonon (DOS) of the Ni/Fe atom at the perfect contact interface is obtained at the average interfacial temperature of 623 *K*, as shown in Figure 4. The phonon frequency of Ni atom at the interface ranges from 0 to10 THz, while the phonon frequency of Fe atom is from 0 to 14.5 THz. The phonons of the Ni and Fe atoms at the interface remain matched in the frequency range of 0～3 THz and 8～10 THz, while the phonons have a significant mismatch in other frequency ranges.

When the interfacial lattice defect concentration is adjusted to 30%, the Ni and Fe atoms are in incomplete contact at the interface and the DOSs of the Ni/Fe atom at the interface are obtained at the average interfacial temperature (the arithmetic mean of the hot and cold zone temperatures) of 623 *K*, as shown in Figure 5. The removal of Ni atoms at contact surface causes the surface lattice defects, reducing the phonon binding probability on both sides of the interface and making the degree of acoustic mismatch worse. At the frequency range of 8-10THz, the phonons no longer match. However, the low-frequency phonons in the range of 0 to 3 THz are almost unaffected by the interfacial lattice defects throughout the heat transfer process. It shows that low-frequency phonon heat transfer is dominant in the interfacial heat transfer. The intermediate or high frequency phonons do not match at the interface, and the degree of mismatch increases with the increase in the interfacial lattice defect

concentration which causes h_{ph} to decrease rapidly. Therefore, to improve the phonon interfacial heat transfer, it is necessary to improve the matching degree of low or intermediate frequency phonons at the interface.

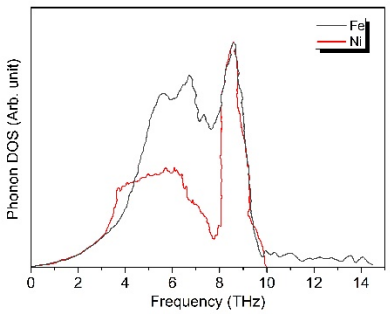


Figure 4. Density of phonon states of Ni and Fe at complete contact interface.

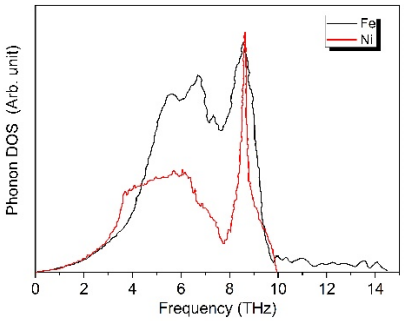


Figure 5. Density of phonon states of Ni and Fe at incomplete contact interface.

3.2.Influence of average temperature of different interfaces on phonon heat transfer coefficient

Figure 6 shows the phonon heat transfer coefficient obtained when the interfacial lattice defect concentration is 5%, the hot zone temperature remains fixed (673 *K*) and the cold zone temperature increases; or the cold zone temperature remains fixed (613 *K*) and the hot zone temperature increases. Here the temperatures of hot and cold zones correspond to the initial forging temperature and the preheating temperature of the billet and the die at the contact surface. When the average interfacial temperature continues to increase, h_{ph} also increases. h_{ph} increases fast at an early stage of heat conduction, then its growth rate is gradually slowed down. It is also observed that if the average temperature of the interface is the same, h_{ph} increases always greater when the temperature of the hot zone remains unchanged and the temperature of the cold zone increases, than that when the temperature of the cold zone remains unchanged and the temperature of the hot zone increases. This indicates that the phonon heat conduction is not sensitive to the temperature change in the hot zone, and the influence of the temperature change in the cold zone on the phonon heat transfer coefficient is more significant.

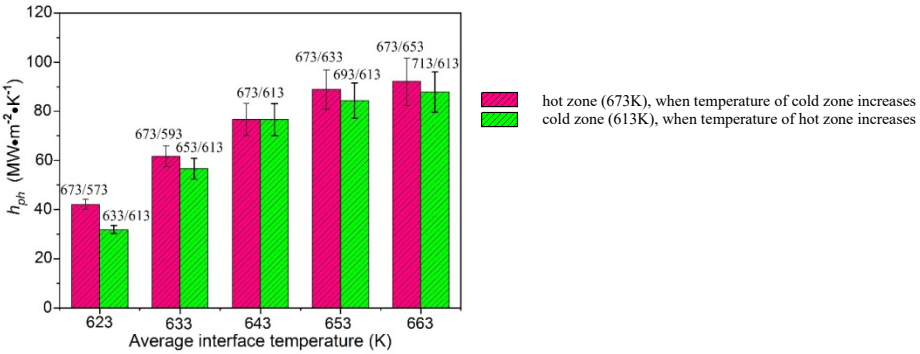
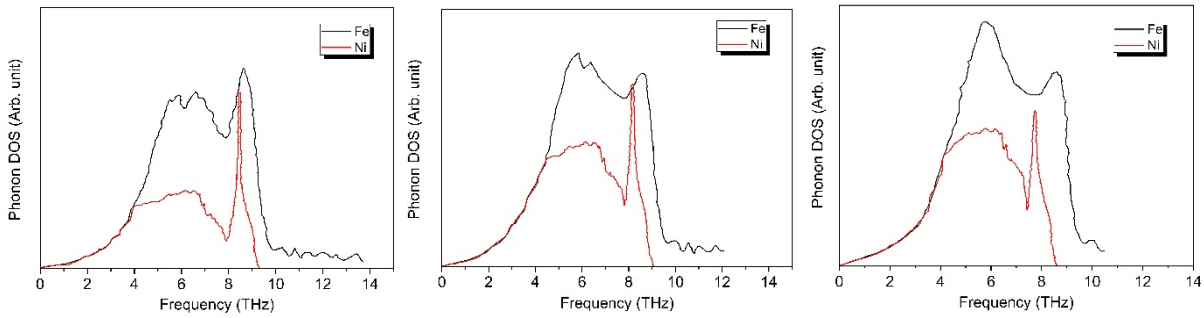


Figure 6.Variation of h_{ph} with different average interface temperature.

The maximum heat transfer coefficient h_{ph} calculated in Figure 6 is 90 MW/(m^{2}K), which is several orders of magnitude higher than the experimental results of the global interfacial heat transfer coefficient (IHTC, [5]). In fact, h_{ph} is part of the IHTC and should be less than the IHTC value. However, in the MD simulation of this example, there are three main reasons for the high phonon heat transfer coefficient h_{ph}: (1) when performing MD simulation, the thickness of the heat conductive layer is only a few nanometers. The surface roughness in the real contact interface during hot forming is at least micron-scale. (2) the non-metallic inclusions are neglected in the MD simulation which may have negative impact on the interfacial heat transfer. (3) the simplified model error and calculation error and their error accumulation.

To further investigate the effect of interfacial temperature changes on the phonon heat transfer coefficient h_{ph}, Figure 7 shows the phonon state density matching curves for Ni/Fe atoms at different average interfacial temperatures when the interfacial lattice defect concentration is 30%. When the average interfacial temperature increases from 623 *K* to 663 *K*, the low-frequency phonon densities of Ni and Fe atoms increase at the interface, and the low-frequency phonon matching degree also increases. The high-frequency phonons and their density peaks continue to decompose during the energy transmission process. As the frequency of high-frequency phonons is continuously attenuated, the frequencies of high-frequency phonons of Ni and Fe atoms are attenuated from 9.25 THz and 13.7 THz at 623 *K* to 8.7 THz and 10.5 THz at 663 *K*, respectively. The peaks of DOS of corresponding to high-frequency phonons also decrease with the increase in the interfacial temperature. At the same time, the intermediate and low frequency phonons increase continuously, so that their phonon density curves are shifted upwards. This shows that high-frequency phonons at high temperature are decomposed during energy transmission, and are decomposed into two or more low-frequency phonons. The latter promotes the matching of low-frequency phonons and increases the probability of phonon transmission at the interface. Therefore, the phonon heat transfer coefficient h_{ph} generally increases with the increase in the interfacial temperature, which explains the basic experimental fact that the IHTC increases with the increase in the interfacial temperature.



(a) 623K (b) 643K (c) 663K

Figure 7. Phonon DOS matching curves of Ni/Fe atom under different average interface temperatures.

4. Conclusions

By use of non-equilibrium molecular dynamics and phonon scattering theory, the phonon heat transfer process at the billet/die imperfect interface at nano-scale is analysed. It is found that when the lattice defect concentration increases, the phonon mismatch at the interface deteriorates and the interfacial thermal resistance increases, which leads to a sharp decrease in phonon heat transfer coefficient. A higher temperature of the contact body and a higher average interfacial temperature result in a higher probability of scattering of phonons at the interface. Moreover, the high frequency phonons at high temperature might be decomposed into low frequency phonons.

5. References

[1] Myers H P 1990 *Introductory Solid State Physics* (London: Taylor & Francis).
[2] Yuan S P and Jiang P Y 2005 *J. Engineering Thermophysics* **A1** 175
[3] Todd B D and Daivis P J 2017 *Nonequilibrium Molecular Dynamics: Theory, Algorithms and Applications* (Cambridge: Cambridge University Press)
[4] Finnis M W and Sinclair J E 1984 *Phil. Mag.* **50** 45
[5] Lu B, Wang L and Huang Y 2016 *Applied Thermal Engineering* **108** 516

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