Thermal Wave Propagation Phenomenon in Thin Film Subjected to Symmetrical Temperature Change

Torii, Shuichi; and Wen-Jei, Yang

Abstract— ***Numerical study is performed on thermal propagation in a very thin film subjected to a symmetrical temperature change on both sides by means of molecular dynamics method. Numerical result is compared with the other numerical one which is obtained from the non-Fourier, hyperbolic heat conduction equation using a numerical technique based on MacCormak's predictor-corrector scheme. Consideration is given to the time history of thermal wave before and after symmetrical collision of wave fronts from both sides of a film. It is disclosed that (i) in transient heat conduction, thermal wave front is transported as a wave in the film, (ii) substantial temperature amplification causes within a very short period of time, and (iii) the heat-affected and undisturbed zones are found to be caused by the atomic movement and in particular the temperature overshoot is induced by the substantial amplification of the atom movement in the film.***

Index Terms— ***molecular dynamics, thermal shock wave, thermal propagation***

1. INTRODUCTION

The classical theory of heat conduction is based on the Fourier's law. This implies that heat conduction in materials is usually treated as a diffusion process in which the effect of a thermal disturbance is transmitted throughout the materials with an infinite velocity. Although infinite transmission speeds and an instantaneous steady-state heat flux are not physically accurate, Fourier's law gives quite reliable results in most practical heat transfer applications. When the elapsed time during a transient is extremely small, the classical Fourier's heat conduction equation breaks down at temperatures near absolute zero or at moderate temperatures. This is because the wave nature of thermal propagation is dominant, that is, a thermal disturbance travels in the medium with a finite speed of propagation [1, 2, 3, 4]. Several issues of basic scientific interest arise in cases such as laser penetration and welding, explosive bonding, electrical discharge machining, and heating and cooling of micro-electronic elements. In particular, the issue of energy transfer into a lattice and resulting temperature in the lattices during such a short period of time and over such a tiny region is of fundamental importance, but remains a matter of controversy [5].

The phenomena are physically anomalous and can be remedied through the introduction of a hyperbolic equation based on a relaxation model for heat conduction which accounts for a finite thermal propagation speed. Recently, considerable interest has been generated toward the hyperbolic heat conduction (HHC) equation and its potential applications in engineering and technology. Some researchers studied wave characteristics and finite propagation speeds in transient heat transfer conduction [3, 6, 7, 8, 9, 10]. Baumeister and Hamill [1] studied thermal wave in a semi-infinite solid subjected to a suddenly applied temperature at the wall. Kao [11] investigated the temperature wave across tin-film media. Carey and Tsai [12] analyzed a one-dimensional case for a propagating heat wave reflected at a boundary. A similar study was carried out by Maurer and Thompson [4], who emphasized the importance of the wave effect in response to a high heat flux irradiation. Glass et al. [13] developed a numerical technique based on MacCormack's predictor-corrector scheme capable of predicting the wave front propagating in materials and its discontinuity. Glass et al. [14] applied the same method to the hyperbolic Stefan problem with a heat flux boundary condition and temperature dependent thermal conduction and obtained the interface position and the temperature distribution in a semi-infinite slab. Frankel et al. [15] developed a general three-dimensional constant property heat flux formulation based on the hyperbolic heat conduction approximation. Tan and Yang [16] investigated heat transfer resulting from a symmetrical collision of thermal waves induced by a step change in the wall temperature of the thin film by means of the method of separation of variables. Results were obtained for the time history of the propagation process, magnitude and shape of the thermal waves, and the range of film thickness and duration time. By using the same method, Tan and Yang [17] predicted the wave

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nature of heat propagation in a very thin film subjected to an asymmetrical temperature change on both sides. Furthermore, Tan and Yang [18] treated heat propagation in a very thin film subjected to an exponentially decaying temperature change on both sides. The corresponding numerical analysis is performed by Torii [19], who employ MacCormak's predictor-corrector scheme to solve the non-Fourier, hyperbolic heat conduction equation. Pulvirenti et al. [20] also investigated a numerical evaluation of the temperature field in an infinite solid medium, in which the thermal conductivity and specific heat of the solid medium are considered as temperature-dependent. The similar problem, i.e., thermal wave propagation phenomena in thin solid films with temperature-dependent thermal conductivity is also studied by Torii and Yang [21].

In general, heat conduction is one of the energy transfer mechanisms of molecules through kinetic motion and potential interaction, while the energy transfer of solid materials will be dominated by potential interaction. Even in molecular collisions, the final process of energy transfer should be controlled by potential interaction. Thus, in order to disclose the detailed physical mechanism of the thermal phenomena, the molecular dynamics method, which solves the movement of atoms or molecules directly without a relation formula between heat flux and temperature, is capable of revealing the thermal propagation phenomena. For example, Kotake and Wakui [22] investigated the process of heat conduction in solid materials by using the molecular dynamics simulation.

This paper treats wave behavior during transient heat conduction in a very thin film (solid plate) subjected to a symmetrical temperature change on both side surfaces. Numerical solutions are obtained by means of the molecular dynamics equation and hyperbolic heat conduction equation. The aim of the study is to compare results of atomistic and HHC macroscopic models. Emphasis is placed on the thermal propagation in the solid medium.

2. Formulation and Numerical Method

2-1 Molecular dynamics equation

Thermal propagation in nanoscale fcc metal (as aluminum) is analyzed. At *t=0*, the temperature within medium is uniform. For *t>0*, two opposite wall sides are suddenly heated at the same temperature. It is assumed that radiation is negligible and there is no effect of the inner heat source. The physical configuration and the coordinate system are shown in Fig. 1.

In molecular dynamics simulation, Newton's equation of motion for atoms or molecules can be written using Hamilton's mechanics relationship as:

$$m_i \frac{d^2\mathbf{r}_i}{dt^2} = \sum_{j\neq i}\mathbf{F}_{ij} = -\frac{d}{dr_{ij}}\sum_{j\neq i}\Phi(\mathbf{r}_{ij}) \ , \qquad (1)$$

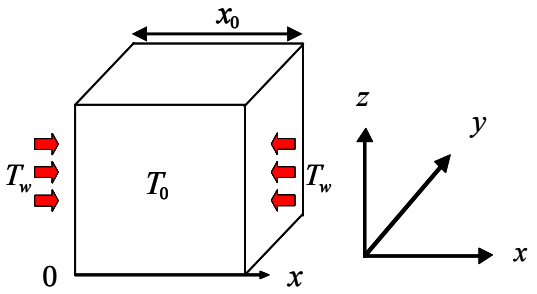


Figure 1. Physical configuration and coordinate system.

where $\mathbf{r}_i$, m_i and $\mathbf{F}_{ij}$ denote the position, mass and force between the particles *I* and *j*, respectively. *t* and $\Phi(\mathbf{r}_{ij})$ represent the time and the potential between two atoms *i* and *j*, respectively. $\mathbf{r}_{ij}$ is the distance between *i* and *j* atoms, i.e., $\mathbf{r}_{ij}=\mathbf{r}_i-\mathbf{r}_j$. In this paper, Morse potential, which is commonly useful for solid-solid metals interaction, is used as a potential function:

$$\Phi(\mathbf{r}_{ij}) = De^{-2A(r_{ij}-r_0)} - 2De^{-A(r_{ij}-r_0)} \ . \qquad (2)$$

Here, D, A, and r_0 are the physical constants. The position and velocity vector of atoms or molecules were solved by Verlet Method, in which the position is determined by a second-order accurate explicit difference equation at 0-1 step as:

$$\mathbf{r}_i(t+\Delta t) = \mathbf{r}_i(t) + \Delta t\mathbf{v}_i(t) + \Delta t^2 a_i(t)/2 \qquad (3)$$

$$\mathbf{r}_i(t+\Delta t) = 2\mathbf{r}_i(t) - \mathbf{r}_i(t-\Delta t) + (\Delta t)^2\sum_{j\neq}\frac{\mathbf{F}_{ij}(t)}{m_i} \qquad (4)$$

$$\mathbf{v}_i(t) = \frac{1}{2\Delta t}\{\mathbf{r}_i(t+\Delta t) - \mathbf{r}_i(t-\Delta t)\} \qquad (5)$$

where, $\mathbf{v}_i$ is the velocity vector in the i direction. The local temperature *T* can be obtained based on the Maxwell's velocity law as:

$$T(t) = \frac{2}{3Nk_B}\left[\frac{1}{2}\sum_{n=1}^{N} m\left\{v_x^2(t)+v_y^2(t)+v_z^2(t)\right\}\right] \qquad (6)$$

where *N* is the atomic number and k_B is the Boltzmann constant k (=1.3805×10-23 [J/K]). Here, N=1,000,000,000 is employed.

Extra spaces are added above and below the target, which allow the macro-motion of atoms in the x direction, as shown in Fig. 1. Periodic boundary conditions are implemented on boundaries in the y and z directions, and free boundary conditions on boundaries in the x direction. The first step of the calculation is to initialize the system to thermal equilibrium before heating start, which is achieved by a thermal

equilibrium calculation. In this calculation, before heating start, the target is initially constructed based on the fcc lattice structure of the aluminum. The values the parameters used in the simulation are listed in Table 1.

Table 1. Parameter of aluminum

D	0.2703	[eV]*
A	1.1646	[Å^{-1}]*
r_0	3.253	[Å]*
m	26.981539/(6.02252×10^{23})	[g]
k_B	1.38062×10^{-23}	[J/K]
s	2.6578	[Å]
r_c	6.6445	[Å]

2-2 Linearized thermal wave theory

Consider a very thin film with thickness of x_0 maintained at a uniform, initial temperature T_0, as mentioned in the above section. The walls at x=0 and x_0 are suddenly heated at a same temperature T_w. Under the conditions, the constitutive equation used in the linearized thermal wave theory [9] is expressed as

$$\tau \frac{\partial q(t,x)}{\partial t} + q(x,t) + k \frac{\partial T(t,x)}{\partial x} = 0 \tag{7}$$

Note that the relaxation time τ defined as $\tau=\alpha/C^2$ is assumed to be constant, where C is the speed of "second sound" (thermal shock wave) and α and k are thermal diffusivity and thermal conductivity, respectively. In the one-dimensional flow of heat, the energy equation in the absence of the heat generation reads:

$$\rho c_p \frac{\partial T(t,x)}{\partial t} + \frac{\partial q(t,x)}{\partial x} = 0 \tag{8}$$

Attention is focused on a film with thickness of x_0 maintained at a uniform, initial temperature T_0. The walls at x=0 and x_0 are suddenly heated with uniform wall temperature. In the present study, radiation is assumed to be negligible. The initial and boundary conditions to be imposed here are given by

$T = T_0$ at t = 0, 0 < x < x_0
$T = T_w$ at t > 0, x = 0 and x = x_0

The following dimensionless quantities are introduced: dimensionless temperature, dimensionless heat flux, and dimensionless time and space:

$$\theta(\xi,\eta) = \frac{T - T_0}{T_W - T_0} \tag{9}$$

$$Q(\xi,\eta) = \frac{\alpha_0 q}{(T_w - T_0) k_0 C_0} \tag{10}$$

$$\xi = \frac{C_0{}^2 t}{2\alpha_0} \tag{11}$$

$$\eta = \frac{C_0 x}{2\alpha_0} \tag{12}$$

Here α_o and C_o is thermal diffusivity and specific heat at initial temperature T_0, respectively. Equations (7) and (8) can be expressed in terms of the above dimensionless variables as:

$$\frac{\partial Q(\xi,\eta)}{\partial \xi} + 2Q(\xi,\eta) + \frac{\partial \theta(\xi,\eta)}{\partial \eta} = 0 \tag{13}$$

and

$$\frac{\partial Q(\xi,\eta)}{\partial \eta} + \frac{\partial \theta(\xi,\eta)}{\partial \xi} = 0 \tag{14}$$

respectively. The initial and boundary conditions become:

θ= 0, Q = 0 at ξ=0, 0<η=η_0
θ= 1.0, $\frac{\partial Q}{\partial \eta} = 0$, at ξ>0, η=0 and η=η_0

where, $\eta_0 = \frac{C_0 x_0}{2\alpha_0}$

Note that the boundary condition of Q at ξ > 0 is derived from Eqs. (7) and (8).

In general, investigators have combined the flux and energy equations (i.e., Eqs. (7) and (8)) into a single second-order partial differential equation to solve the HHC problem. For this solution method, Glass et al. [13] disclosed that MacCormack's method [23], which is a second-order accurate explicit scheme, can handle these moving discontinuities quite well and is valid for HHC problems. The hyperbolic problems considered in the present study have step discontinuities at the thermal wave front. MacCormack's prediction-correction scheme is therefore used. When the HHC problem is numerically solved through the scheme employed here, it is convenient to solve Eqs. (7) and (8) separately rather than combining them into a single second-order partial differential equation [13]. When MacCormack's method is applied to Eqs. (10) and (11), the following finite difference formulation results:

Predictor:

$$\overline{\theta_i^{n+1}} = \theta_i^n - \frac{\Delta\xi}{\Delta\eta}\left(Q_{i+1}^n - Q_i^n\right) \tag{15}$$

$$\overline{Q_i^{n+1}} = Q_i^n - \frac{\Delta\xi}{\Delta\eta}\left\{\theta_{i+1}^n - \theta_i^n\right\} - 2\Delta\xi\, Q_i^n \tag{16}$$

Corrector:

$$\theta_i^{n+1} = \frac{1}{2}\left\{\theta_i^n + \overline{\theta_i^{n+1}} - \frac{\Delta\xi}{\Delta\eta}\left(\overline{Q_i^{n+1}} - \overline{Q_{i-1}^{n+1}}\right)\right\} \quad (17)$$

$$Q_i^{n+1} = \frac{1}{2}\left[Q_i^n + \overline{Q_i^{n+1}} - \frac{\Delta\xi}{\Delta\eta}\left\{\overline{\theta_i^{n+1}} - \overline{\theta_{i-1}^{n+1}}\right\} - 2\Delta\xi\overline{Q_i^{n+1}}\right] \quad (18)$$

Here, the subscript i denotes the grid points in the space domain, superscript n denotes the time level, and $\Delta\eta$ and $\Delta\xi$are the space and time steps, respectively. The circumflex terms, i.e., $\overline{Q_i^{n+1}}$, $\overline{\theta_i^{n+1}}$, etc. are a temporary predicted value at the time level n+1.

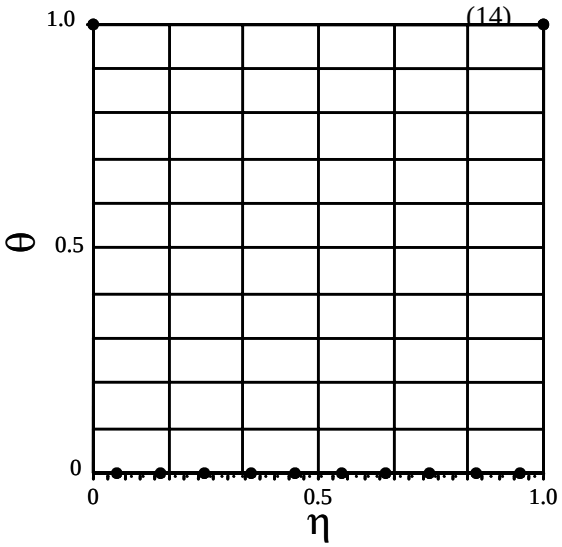
Computations are processed in the following order:

1. Specify the values of Q and θ at ξ=0, i.e., the initial values.
2. Solve Eqs. (15) and (16) for θ and Q to obtain temporary predicted value at the time level n+1.
3. Calculate new values of θ and Q at the time step n+1 using Eqs. (17) and (18).
4. Repeat steps 2-3 until n reaches a desired time level from the onset of calculation.

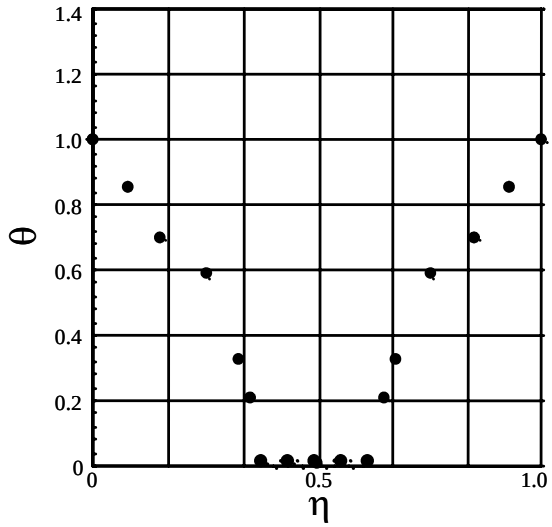
Throughout numerical calculations, the number of grids is properly selected between 1,000 and 5,000 to obtain a grid-independent solution. This results in no appreciable difference between the numerical results with different grid spacing, in which the dimensionless temperature distributions in a film are depicted with different grid size, as the parameter. In solving the governing equations employed here, i.e., the HHC problem including the nonlinear nature, the stability is affected by the ratio of $\Delta\xi$ to $\Delta\eta$, $\Delta\xi/\Delta\eta$, which is called the Courant number [24]. For example, as the Courant number becomes smaller, the effect of odd derivative truncation-error terms becomes larger, and oscillations occur in the vicinity of discontinuities in the solution. Therefore, $\Delta\xi/\Delta\eta$ is fixed at 0.98 in the present study.

3. RESULTS AND DISUCUSSION

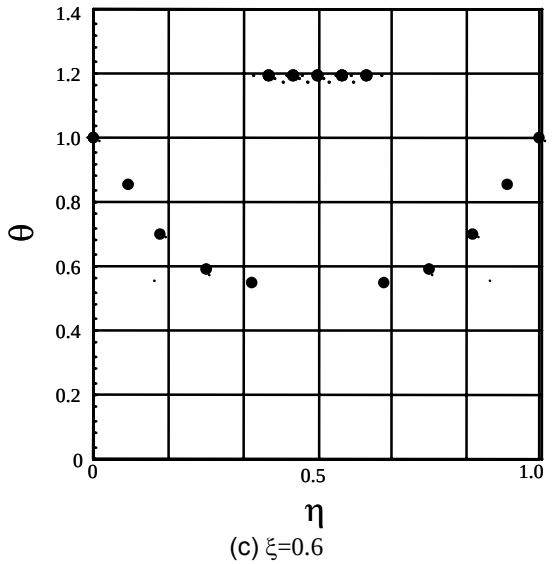
Figure 2 illustrates the temperature distribution in the film at different time. Here, the solid circle implies the temperature at the molecular location used here, but all molecular locations are not shown. One observes that after the wall temperature on two sides is suddenly raised, the film temperature is increased as time progresses and there are the area of the temperature amplification and its no effect area in the film. This implies that a thermal disturbance is transmitted throughout the film with a finite velocity, whose nature can not be predicted by the Fourier's law. In other words, the thermal propagation is in contrast to the diffusion nature, which is dominated based on the Fourier's law. It should be noticed that the film temperatures in the vicinity of both sides of strongly heated walls exceed the imposed wall temperature at ξ=0.6, as seen in Fig. 2(c). These temperature characteristics become clearer for the atomic behavior in the film.



(a) ξ=0.0

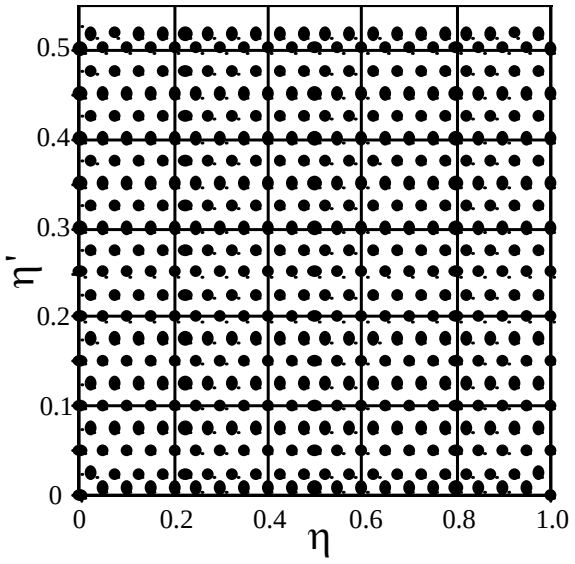


(b) ξ=0.4

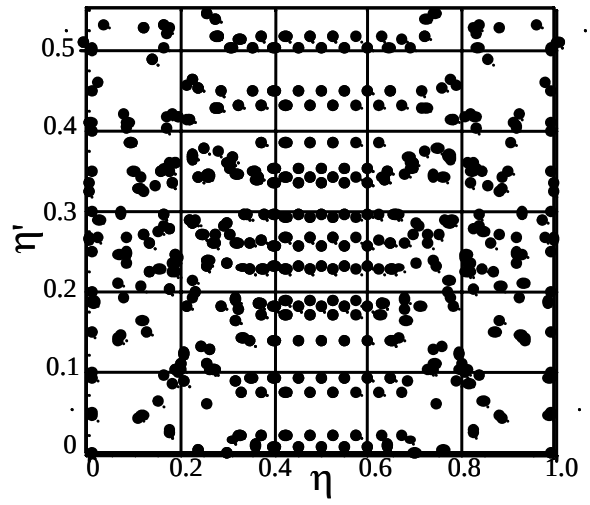


(c) ξ=0.6

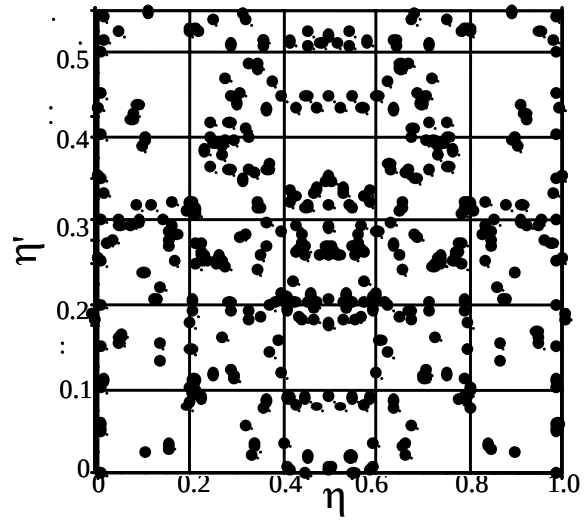
Figure 2. Temperature distribution in the thin film.



(a) ξ=0.0



(b) ξ=0.4



(c) ξ=0.6

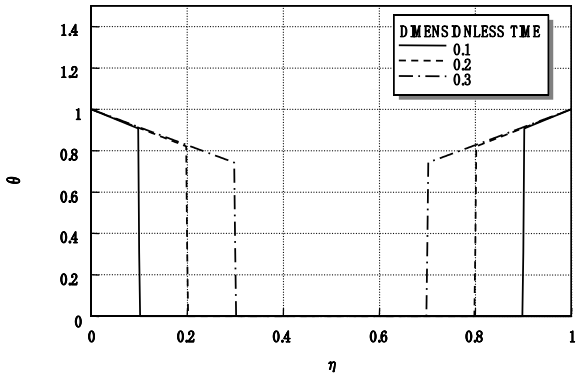
Figure 3. Atomic behaviour in thin film.

The corresponding atom distribution is depicted in Fig. 3 with the initial atomic location shown in Fig. 3(a) for reference. Notice that all atom locations are not depicted in Fig. 3, because the atom movement becomes clearer. Here, $\eta'=C_0z/2\alpha_0$ and the atomic location implies the average value along y axis at each η location. It is observed that at ξ=0.4, the atoms move near both heated side walls, while no movement of the atoms appears in the central zone of the film. At ξ=0.6, the substantial movement of the atoms yields over the whole file area, resulting in occurrence of the temperature overshoot, as seen in Fig. 2(c).

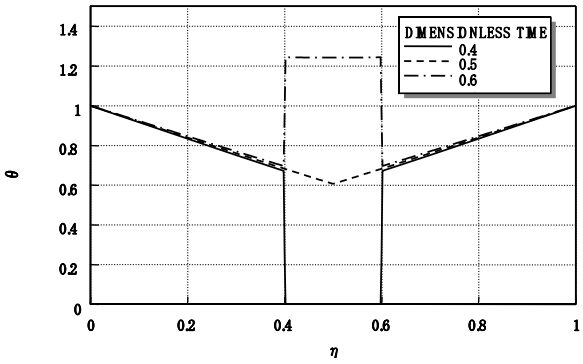
Figures 4(a) and (b) illustrate the timewise variation of the temperature distribution, θ, in a film having η=1. They are obtained by means of a numerical technique based on MacCormak's predictor-corrector scheme to solve the non-Fourier, hyperbolic heat conduction equation and correspond to numerical predictions before and after collision of thermal wave fronts, respectively. Note that Fig. 4 reproduces precisely the theoretical results of Tan and Yang [17], which show in detail the propagation process of thermal waves in a film. Figure 4(a) depicts that after the wall temperatures on both sides are suddenly raised, a set of sharp wavefronts appears in the thermal wave propagation and advances towards the center in the physical domain which separates the heat-affected zone from the thermally undisturbed zone. Here both zones are caused by the active movement and no movement of the atoms, as seen in Fig. 3(b). It is observed in Fig. 4(b) that after first collision, the center temperature in a film causes a significant amplification, resulting in much higher temperature in this region, which is induced by the substantial movement of the atoms (Fig. 3(c)). A temperature overshoot is predicted by the molecular dynamic simulation, as shown in Fig. 2(c). The numerical solution predicts the existence of thermal waves, particularly in a very thin film and presents the propagation process of thermal waves, the magnitude and shape of thermal waves.

4. SUMMARY

It is revealed that if a film is strongly heated, a temperature overshoot takes place in the film of smaller thickness within a very short period of time. The transient temperature distribution is simulated for heat conduction process in nano-scale structure using the molecular dynamics equation and hyperbolic heat conduction equation, that is by means of atomistic and HHC macroscopic models. The heat-affected and undisturbed zones are found to be caused by the atomic movement and in particular the temperature overshoot is induced by substantial amplification of the atom movement in the film.



(a) Before collision of thermal wavefronts



(b) After collision of thermal wavefronts

Figure 4. Temperature distribution predicted by non-Fourier, hyperbolic heat conduction equation.

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