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Study on thermal wave based on the thermal mass theory

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The conservation equations for heat conduction are established based on the concept of thermal mass. We obtain a general heat conduction law which takes into account the spatial and temporal inertia of thermal mass. The general law introduces a damped thermal wave equation. It reduces to the well-known CV model when the spatial inertia of heat flux and temperature and the temporal inertia of temperature are neglected, which indicates that the CV model only considers the temporal inertia of heat flux. Numerical simulations on the propagation and superposition of thermal waves show that for small thermal perturbation the CV model agrees with the thermal wave equation based on the thermal mass theory. For larger thermal perturbation, however, the physically impossible phenomenon predicted by CV model, i.e. the negative temperature induced by the thermal wave superposition, is eliminated by the general heat conduction law, which demonstrates that the present heat conduction law based on the thermal mass theory is more reasonable.

thermal wave, thermal mass theory, non-Fourier heat conduction, CV model

In the classical theory of heat transfer, the law established by Joseph Fourier, a French physical and mathematical scientist, in 1822 is basicly used to characterize heat conduction[1]

$$q = -k\nabla T, \tag{1}$$

where q is the heat flux, T is the temperature and k is the thermal conductivity. The Fourier's law leads to a parabolic and diffusive governing equation for the temperature field, which implies that the propagation velocity of a thermal perturbation is infinite. For normal conditions, the Fourier's heat conduction law agrees with the experimental results very well. However, with the rapid advancement of modern experimental technologies, the Fourier's law is found to fail in ultralow temperature and transient heat transport processes, where the thermal perturbation propagates like waves and with finite velocity. It is called thermal wave[2,3].

Tisze (1938)[4] and Landau (1941)[5] respectively predicted the possible wave-like heat propagation in helium II with finite speed, which is similar to a sound wave induced by pressure perturbation. This effect caused by the thermal pertubation is called "second sound". Several years later, Peshkov[6] validated the prediction in his famous experiments. He measured the velocity of the thermal wave propagation in helium II about 19 m/s at 1.4 K, which is one order of magnitude less than the speed of sound in helium II. Brorson et al.[7] measured the interval of thermal pulses passing through metallic films and confirmed the existence of the thermal wave. However, the experimental meansurements on the thermal wave phenomenon were quite rare due to the tremendous technological difficulty.

In order to interpret the thermal wave phenomenon, Cattaneo in 1948[8] and Vernotte in 1958[9] modified the Fourier's heat conduction law respectively

$$q + \tau\frac{\partial q}{\partial t} = -k\nabla T, \tag{2}$$

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in which q is the heat flux, ∇T is the gradient of temperature, k is the thermal conductivity, t is time and τ is the relaxation time which is usually less than 10^{-11} s. Eq. (2) is just the well-known CV model. The governing equation for temperature fields based on CV model can be written as

$$\frac{\partial T}{\partial t}+\tau\frac{\partial^2 T}{\partial t^2}=a\nabla^2 T, \tag{3}$$

where $a=k/\rho c_v$ is the thermal diffusivity. Since the equation is hyperbolic, the propagation velocity of a heat perturbation becomes finite. The thermal energy transport is predicted as wave propagation by the CV model rather than diffusion by the Fourier's law. As the realxation time, τ, is very small, the CV model of eq. (2) can reduce to the Fourier's law, i.e. eq. (1), for normal conditions. When the heat flux varies very fast (e.g. a laser heat pulse), however, the characteristics of wave propagation will dominate the thermal transport process.

Many theoretical analyses and numerical simulations on transient heat transport based on the CV model have been performed by many reserachers, such as Xu and Guo[10], Antaki[11], Cho and Juhng[12], Fan and Lu[13], and Zhang et al.[14], Tang and Araki[15] put forward a method for measuring the thermal relaxation time. Recently, Bai and Lavine[16] and Körner et al.[17] pointed out that the CV model might result in a physically impossible phenomenon of negative temperature during thermal wave superpositions.

The derivative of heat flux to time in the CV model essentially means the variation of heat flux is later than the establishment of temperature gradient, which implies thermal inertia. In 1917 Nernst[18] predicted that thermal oscillations could be caused by the large thermal inertia in good thermal conductors at low temperature. In 1931, Onsager[19] indicated that the Fourier's heat conduction law had neglected the time for the heat flux to accelerate, which also implied the inertial effect of heat conduction. Actually the inertia is characterized by the mass of an object, though thermal energy is traditionally incompatible with mass. Until recently, Guo et al.[20−22] introduced Einstein's mass-energy relation to phonon gas theory and proposed a new concept called thermal mass. In the theory of thermal mass, the mass of thermal energy is equal to the ratio of the thermal energy to the squared speed of light in vacuum. They established the conservation equations for the motion of the thermal mass based on Newtonian mechanics. Thus, the wave-like effects on heat transport could be investigated based on these conservation equations. In this paper, the thermal wave phenomenon is studied by establishing the governing equations based on the thermal mass theory. The derived heat conduction equation is normally a damped wave model. Numerical simulations on the thermal wave propagation are then performed, and the results show that the thermal mass equation can conquer the physical drawback of the negative temperature in the CV model.

1 Governing equations for thermal wave based on thermal mass theory

According to the Einstein's theory of relativity, the mass and energy of an object are equivalent through the mass-energy relationship. In the theory of thermal mass[20−22], the equivalent mass of thermal energy can be defined by the mass-energy relationship. The thermal mass density can be written as

$$\rho_h=\frac{\rho c_v T}{c^2}, \tag{4}$$

in which ρ_h is the thermal mass density, ρ is the mass density of the object, c_v is the specific heat, and c is the speed of light in vacuum. When there is a temperature gradient in an object, heat flows from high to low temperature, which indicates that the thermal mass drifts at a certain velocity. The velocity of the thermal mass can be derived by the heat flux

$$q_h=\rho_h u_h \text{ or } \quad q=\rho c_v T u_h, \tag{5}$$

where $q_h=q/c^2$ is the thermal mass flux, u_h is the drift velocity of the thermal mass and q is heat flux. The heat conduction can then be investigated using the governing equations for the motion of thermal mass like in fluid dynamics.

Consider a one-dimensional heat conduction in a uniform conductor as shown in Figure 1. The continuity equation for the thermal mass is as follows

$$\frac{\partial \rho_h}{\partial t}+\frac{\partial q_h}{\partial x}=0. \tag{6}$$

Substituting eqs. (4) and (5) into eq. (6) gives

$$\rho c_v\frac{\partial T}{\partial t}+\frac{\partial q}{\partial x}=0. \tag{7}$$

Eq. (7) is actually the conservation equation of thermal energy, which is equivalent to the continuity equation for thermal mass.

For the differential element as shown in Figure 1,

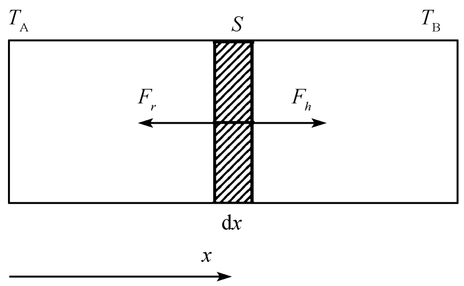

Figure 1 Schematic of the transport process of the thermal mass.

there are a driving force dF_h induced by pressure difference, a resistant force dF_r blocking the motion of the thermal mass, and an inertial force dF_i counteracting the thermal mass acceleration:

$$\mathrm{d}F_h = \frac{\mathrm{d}p_h}{\mathrm{d}x}\mathrm{d}V = -2\gamma\rho_h c_v \frac{\mathrm{d}T}{\mathrm{d}x}\mathrm{d}V, \tag{8a}$$

$$\mathrm{d}F_r = -\xi_h u_h \rho_h \mathrm{d}V, \tag{8b}$$

$$\mathrm{d}F_i = \frac{D(\rho_h u_h)}{Dt}\mathrm{d}V = \left(\frac{\partial(\rho_h u_h)}{\partial t} + u_h \frac{\partial(\rho_h u_h)}{\partial x}\right)\mathrm{d}V, \tag{8c}$$

where γ is the Grüneisen constant. The resistant force is proportional to the drift velocity of the thermal mass with the linear coefficient ζ_h. The inertial force is determined by two parts: One is the temporal inertia caused by the variation of the thermal mass velocity with time; the other is the spatial inertia arising from the accelleration of the thermal mass long a spatial distance. According to the Newton's second law, dF_i=dF_h+dF_r, we can obtain

$$\frac{\partial(\rho_h u_h)}{\partial t} + u_h \frac{\partial(\rho_h u_h)}{\partial x} = -2\gamma\rho_h c_v \frac{\partial T}{\partial x} - \xi_h \rho_h u_h. \tag{9}$$

This is just the momentum conservation equation for the motion of the thermal mass.

With the inertial force being neglected, eq. (9) reduces to the Fourier's heat conductoin law. When the inertial force can not be neglected, the Fourier's law breaks down, which is often called non-Fourier heat conduction. From this point of view, the Fourier's law reflects the balance between the resistant and driving forces of the thermal mass.

Neglecting the inertial force, we can rewrite the momentum conservation equation as

$$2\gamma c_v \frac{\partial T}{\partial x} + \xi_h u_h = 0. \tag{10}$$

According to the Fourier's law, it follows that

$$\xi_h = \frac{2\gamma c^2 \rho_h^2 c_v}{k}. \tag{11}$$

Considering eqs. (4), (5), (9) and (11), we can obtain

$$q + \tau\left(\frac{\partial q}{\partial t} + u_h \frac{\partial q}{\partial x}\right) - \tau u_h \left[\frac{\partial(\rho c_v T)}{\partial t} + u_h \frac{\partial(\rho c_v T)}{\partial x}\right] = -k\frac{\partial T}{\partial x}, \tag{12}$$

where $\tau = a/(2\gamma c_v T)$ is the characteristic time. For normal conditions, the characteristic time is on the order of $10^{-10}-10^{-14}$ s, the same order as the relaxation time in the CV model. The thermal wave phenomenon becomes dominant only if the variation rate of the heat flux is of the same order. Different from the relaxation time in the CV model, the characteristic time here represents the medium resistance imposing on the thermal mass and is determined by the physical properties and temperature of materials. Eq. (12) is just a general heat conduction law based on the theory of thermal mass because the derivation of the equation does not have any assumptions. The general law is a hyperbolic equation, which introduces a damped wave equation of temperature. The first term on the left of eq. (12) represents the resistant force, the right of eq. (12) represents the driving force, and other four terms represent the inertial forces.

The four inertial force terms in eq. (12) can be classified into two parts: one represents the temporal inertia of the heat flux and temperature: $\tau\,\partial q/\partial t$ and $\tau\left[u_h\,\partial\left(\rho c_v T\right)/\partial t\right]$; the other represents the spatial inertia: $\tau u_h\,\partial q/\partial x$ and $\tau u_h\left[u_h\,\partial\left(\rho c_v T\right)/\partial x\right]$. By comparing eq. (12) with eq. (2), we can find that the present general heat conduction law will reduce to the CV model when the spatial inertia of the heat flux and temperature and temporal inertia of temperature are all neglected. This indicates that the CV model only takes into account the temporal inertia of the heat flux. This simplification is acceptable for the CV model when the temperature gradient is not very large. Contrarily, the effects of the temporal inertia of the heat flux and temperature become so significant that the CV model breaks down and the general law should be applied.

2 Numerical simulations on thermal wave propagation

Consider one-dimensional thermal wave propagation as shown in Figure 2. The lengths of the simulated system in the y and z directions are infinite. The length in the x

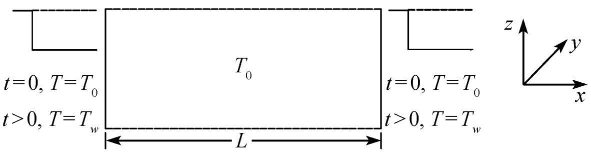

Figure 2 Schematic of thermal wave propagation.

direction is L. The initial temperature in the system is uniform, i.e. T_0. After the initial time, the temperature of the left and right boundaries falls down to a lower temperature, T_w. Thus, the thermal perturbations at the two boundaries will result in two thermal waves propagating and superposing inside the object.

2.1 Numerical method for CV model

For simplicity, dimensionless units are used

$$t^* = \upsilon^2 t / a\,,\quad x^* = \upsilon x / a\,,\quad T^* = T / T_0\,,$$

where $\upsilon = \sqrt{a/\tau}$, t^*, x^* and T^* are the dimensionless time, coordinate and temperature, respectively. Substituting the dimensionless parameters into eq. (2) together with eq. (7), we get the dimensionless equation of heat conduction based on the CV model:

$$\frac{\partial^2 T^*}{\partial t^{*2}} + \frac{\partial T^*}{\partial t^*} = \frac{\partial^2 T^*}{\partial x^{*2}}. \tag{13a}$$

The initial conditions can be written as

$$T^*(x^*,0) = 1\,,\quad \frac{\partial T^*}{\partial t^*}(x^*,0) = 0\,, \tag{13b}$$

and the boundary conditions are

$$T^*(0,t^*) = T^*(1,t^*) = 1 + A, \tag{13c}$$

where $A = (T_w - T_0)/T_0$.

The closed equations for solving the dimensionless CV model numerically can then be obtained by discretizing eq. (13a) using central difference for spatial discretization and backward difference for temporal discretization.

2.2 Numerical method for thermal mass equation

Since there are two variables in eq. (12), i.e. the temperature T and the heat flux q, to close the equations should solve the continuity equations simultaneously. Eq. (12) is equivalent to eqs. (6) and (9). Thus, we can solve eqs. (6) and (9) numerically to obtain the temperature distributions varying with time.

The initial heat flux is zero due to the uniform temperature distribution, i.e. $q|_{t=0} = 0$. Using eq. (7) at the boundary with $\frac{\partial T}{\partial t}|_w = 0$, we have $\frac{\partial q}{\partial x}|_w = 0$. The thermal mass equations with the initial boundary conditions for the thermal wave propagation can then be written as

$$\begin{aligned}
&\rho c_v \frac{\partial T}{\partial t} + \frac{\partial q}{\partial x} = 0,\\
&\frac{\partial q}{\partial t} + \frac{q}{\rho c_v T}\frac{\partial q}{\partial x} + \rho c_v^2 T \frac{\partial T}{\partial x} + \frac{\rho c_v^2 T q}{k} = 0,\\
&x = 0:\ T = T_w\,,\ \frac{\partial q}{\partial x} = 0,\\
&x = L:\ T = T_w\,,\ \frac{\partial q}{\partial x} = 0,\\
&t = 0:\ T = T_0 (T_0 > T_w)\,,\ q = 0.
\end{aligned} \tag{14a}$$

Letting $t^* = t/(L^2/a)$, $x^* = x/L$, $T^* = T/T_0$, $q^* = q/(\rho a c_v T_0 / L)$ and substituting them to eq. (14a), we can get the following dimensionless equations

$$\begin{aligned}
&\frac{\partial T^*}{\partial t^*} + \frac{\partial q^*}{\partial x^*} = 0,\\
&\frac{\partial q^*}{\partial t^*} + \frac{q^*}{T^*}\frac{\partial q^*}{\partial x^*} + T^* \frac{\partial T^*}{\partial x^*} + q^* T^* = 0,\\
&x^* = 0:\ T^* = \frac{T_w}{T_0} = 1 + A\,,\ \frac{\partial q^*}{\partial x^*} = 0,\\
&x^* = 1:\ T^* = \frac{T_w}{T_0} = 1 + A\,,\ \frac{\partial q^*}{\partial x^*} = 0,\\
&t^* = 0:\ T^* = 1\,,\ q^* = 0.
\end{aligned} \tag{14b}$$

The closed equations for solving the dimensionless thermal mass model numerically can then be obtained by discretizing eq. (14b) using central difference for spatial discretization and forward difference for temporal discretization.

3 Results and discussion

For the propagation and superposition of thermal waves as shown Figure 2, we solve the thermal mass equation and CV model with $T_w^* = 0.9$, $T_w^* = 0.5$, and $T_w^* = 0.3$, respectively.

With T_w^*=0.9 (A= –0.1), Figure 3 shows the temperature distributions predicted by the CV model and thermal mass equation at the time 0.1, 0.4, 0.8 and 1.2, respectively. The two thermal perturbations at the boundaries lead to two thermal waves as predicted by both

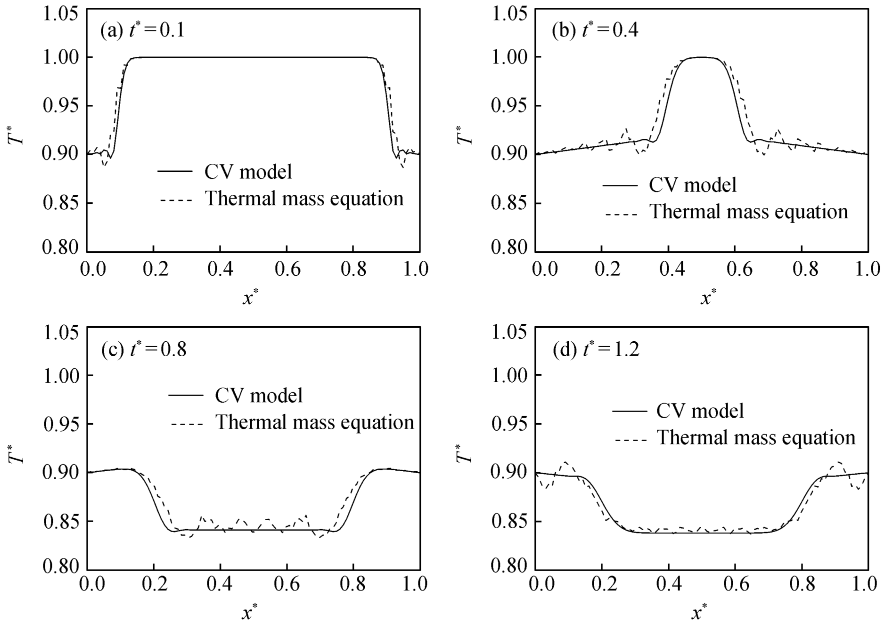

Figure 3 Temperature distribution variations with time (T_w*=0.9).

the CV model and thermal mass equation. Two temperature peaks can be found to move inside the system from the boundaries due to the sudden drop of the boundary temperature. They meet each other and result in superposition as shown in Figure 3(c). We can find that the results obtained by the thermal mass equation and CV model are very close for the dimensionless velocity of the temperature peaks and the temperature distributions. It should be pointed out that the slight fluctuations of the numerical results calculated by the thermal mass equation are due to the explicit scheme of eq. (14b). When the thermal perturbation and heat flux are small such that the spatial inertia of the heat flux can be neglected, the results by the CV model compare with those by the thermal mass equation very well.

Figure 4 shows the temperature distributions respec-

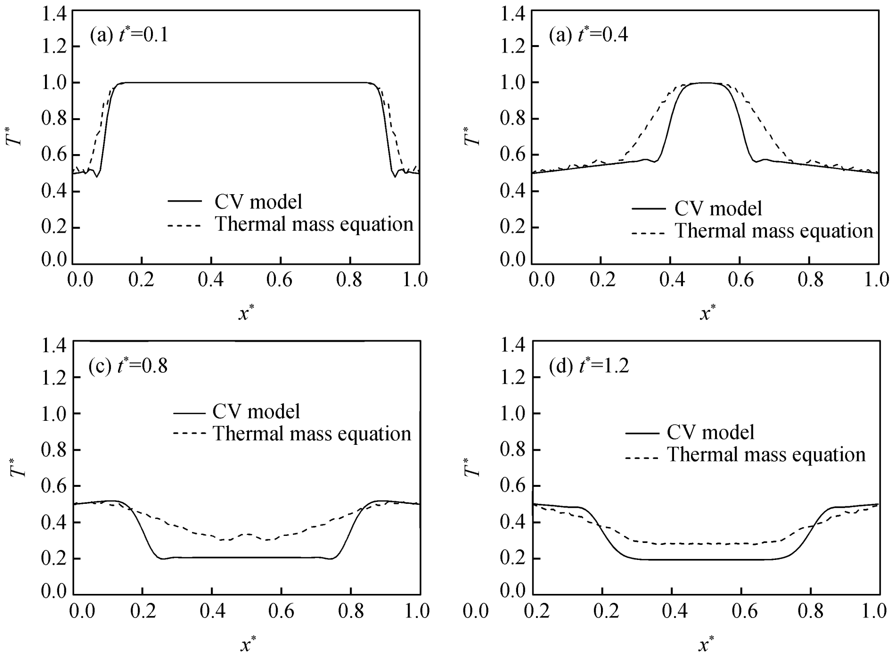

Figure 4 Temperature distribution variation with time (T_w*=0.5).

tively calculated by the CV model and thermal mass equation at the time 0.1, 0.4, 0.8 and 1.2 with T_w^*=0.5 (A = −0.5). The dimensionless velocities of the thermal perturbation predicted by the CV model and thermal mass equation are very close. When the thermal wave peaks meet and overlap, neither of the two models predict the physically impossible solution of negative temperature at the moment. However, the temperature distribution of the thermal wave fronts predicted by the CV model is steeper than that predicted by the thermal mass equation. When the superposition takes place as shown in Figure 4(c), the temperature at the middle of the system predicted by the thermal mass equation is a little higher than that by the CV model. In other words, the temperature drop based on the thermal mass theory is slower than that predicted by the CV model. The reason is that the increase of the heat flux needs to overcome the spatial inertia of the thermal mass motion based on the thermal mass theory.

With T_w^*=0.3 (A=−0.7), Figure 5 shows the temperature distributions predicted by the CV model and thermal mass equation at the time 0.1, 0.4, 0.8 and 1.2, respectively. The dimensionless propagation velocities of the thermal waves obtained by the CV model and thermal mass equation are almost the same. The temperature distributions of the thermal wave fronts predicted by the CV model are also steeper than those by the thermal mass equation. When the two thermal waves meet and overlap, however, the temperature at the middle of the system predicted by the thermal mass equation is much higher than that by the CV model. The prediction calculated by the CV model shows that the temperature would become negative at the moment of two temperature peaks' superposition as shown in Figures 5(c) and (d), which is a physically impossible phenomenon. This indicates that the CV model has great defects to describe the thermal wave propagation with large thermal perturbation as reported in ref. [16]. For the thermal mass equation that considers more inertial forces, the physically impossible phenomenon of negative temperature is conquered under the same conditions. It indicates that by overcoming the non-physical defects of the CV model, the thermal mass equation is better than the CV model when describing the thermal wave propagation with large thermal perturbation.

4 Conclusions

1) The conservation equations for heat conduction are established based on the thermal mass theory. The momentum conservation equation, which considers the inertial forces of heat flux and temperature, is just a general heat conduction law. The general law reduces to the Fourier's heat conduction law if all the inertial forces are neglected. The physical essence of the Fourier's law is the balance between the driving and resistant forces. The

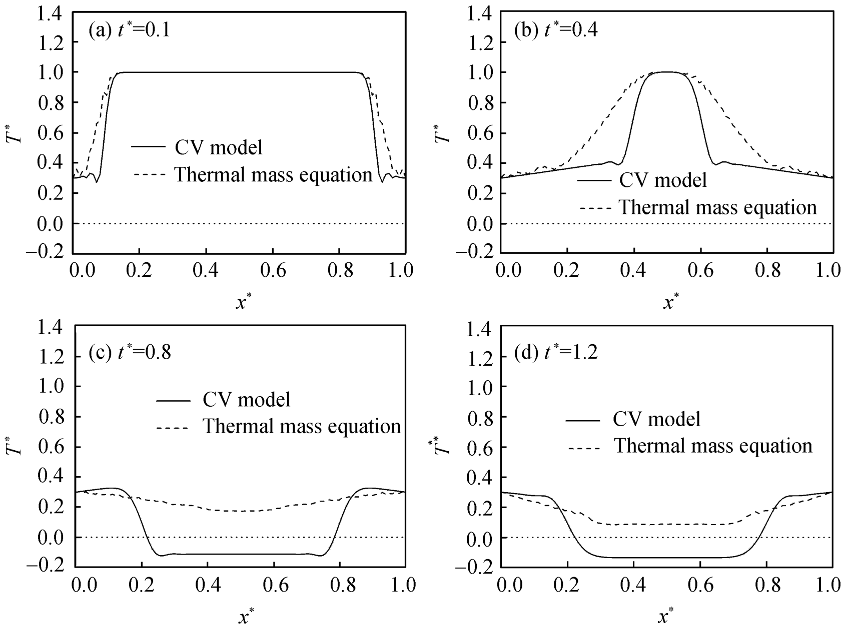

Figure 5 Temperature distribution variations with time (T_w*=0.3).

non-Fourier heat conduction is essentially caused by the inertial effects.

2) The heat conduction law based on the thermal mass theory has four inertial terms of both heat flux and temperature to time and space, respectively. With the spatial inertia of the heat flux and temperature and the temporal inertia of temperature being neglected, the general law reduces to the CV model, which indicates that the CV model just considers the temporal inertia of the heat flux.

3) When the thermal perturbation and heat flux are small such that the spatial inertia of the heat flux can be neglected, the thermal wave behaviors predicted by the thermal mass equation agree with the CV model very well. For the larger thermal perturbation, however, the CV model predicts a physically impossible phenomenon of negative temperature during the superposition of thermal waves. The thermal wave equation based on the thermal mass theory conquers this defect. Numerical simulations show that the thermal mass equation is more physically reasonable than the CV model.

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