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A non-local constitutive model for nano-scale heat conduction

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ABSTRACT

In this article a constitutive model for the nano-scale heat conduction is proposed by accounting for both the spatially and temporally non-local effects. Based on this model the heat conduction of the silicon thin film is investigated. The derived effective thermal conductivity and conductance of the silicon thin films shows a good agreement with the experimental and numerical results. Also derived is the condition for the thermal oscillation of the nano-scale heat conduction.

1. Introduction

We start with the Fourier law, a fundamental law in the heat transfer theory. It is mathematically expressed as follows:

$$\mathbf{q}(\mathbf{r}, t) = -k\nabla T(\mathbf{r}, t) \tag{1}$$

where $\mathbf{r}$ is the position vector, t is the time variable, $\mathbf{q}(\mathbf{r}, t)$ is the heat flux, $\nabla T(\mathbf{r}, t)$ is the temperature gradient, k is the thermal conductivity. It is no doubt that the Fourier law has achieved great successes in solving various macro-scale heat transfer problems. However, the rapid developments of the nanotechnology and ultra-fast laser heating technology bring us more and more nano-scale heat conduction problems which challenge the classical Fourier law. Actually, it is well-recognized that the classical Fourier law is inappropriate to heat transports occurring in times comparable to the mean-free time [1–6] where the finite heat transport speed should be considered or in sizes comparable to the mean-free path of energy carriers where the non-local effect can not be neglected [7–12]. Therefore, it is of great importance to modify the Fourier law and develop the constitutive models for nano-scale heat conduction to reflect the non-local and memory effect. In order to avoid the infinite speed of heat propagation which is inferred from the classical Fourier law, Cattaneo and Vernotte proposed the following heat conduction model [13–15]:

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

where τ is the relaxation time, and it is usually called the CV model. The natural extension of this model is

$$\mathbf{q}(\mathbf{r}, t+\tau) = -k\nabla T(\mathbf{r}, t) \tag{3}$$

which is called the single-phase-lagging heat conduction model. The model (3) was further extended to the following dual-phase-lagging heat conduction model by Tzou [1]:

$$\mathbf{q}(\mathbf{r}, t+\tau_q) = -k\nabla T(\mathbf{r}, t+\tau_T) \tag{4}$$

where τ_q and τ_T are the phase lags of the temperature gradient and the heat flux vector, respectively. The first order Taylor expansion of Eq. (4) yields

$$\mathbf{q}(\mathbf{r}, t) + \tau_q\frac{\partial \mathbf{q}(\mathbf{r}, t)}{\partial t} = -k\left[\nabla T(\mathbf{r}, t) + \tau_T\frac{\partial \nabla T(\mathbf{r}, t)}{\partial t}\right] \tag{5}$$

The models (2)–(5) usually give rise to the wave-like behavior of heat transport [1,16–20], thus avoids the infinite heat propagation speed of the classical heat conduction. However, they can not reflect the spatially non-local effect of nano-scale heat conduction, such as the size effect which has been observed experimentally [8–12]. It is well-known that Guyer-Krumhansl model accommodates both the lagging and non-local effects [21–26], which reads

$$\tau\frac{\partial \mathbf{q}}{\partial t} + \mathbf{q} = -k\nabla T + l^2(\Delta\mathbf{q} + 2\nabla\nabla\cdot\mathbf{q}) \tag{6}$$

where l is the mean-free path of phonons, Δ is the Laplace operator. Recently, by taking into account the mass, pressure, and inertial force of the phonon gas, Cao and Guo derived the equation of motion of the phonon gas which leads to the thermomass model for phonon transports [27]. Tzou and Guo generalized the dual-phase-lagging heat conduction model by accounting for the non-local effect in space, which is formulated as follows [28,29]:

$$\mathbf{q}(\mathbf{r}+\mathbf{L}, t+\tau_q) = -k\nabla T(\mathbf{r}, t+\tau_T) \tag{7}$$

where $\mathbf{L}$ is a displacement vector reflecting the spatially non-local effect. Note that if replacing the left side term with its Taylor series at the point $\boldsymbol{r}$, then one can see that the spatially non-local effect is described by the spatial derivatives of the heat flux. Sobolev proposed the two-

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temperature model to study the non-local effect of the heat conduction [30–32]. The extended irreversible thermodynamics has been widely applied in investigating the nano-scale heat conduction problems [33–36].

Interestingly, the fractional dynamics is also employed to investigate the non-local transport phenomena. Recently, Mongioví and Zingales [37] extended the fractional-order thermodynamics [38] and established a fractional-order temperature equation for the non-local thermal energy transport. The fractional calculus was employed to study the non-local mass and heat transport problems [39,40]. The heat and mass transfer in the boundary layer of the fractional MHD Maxwell flow in a porous medium was investigated numerically [41]. Zhao et al. applied the fractional calculus in investigating the natural convection heat transfer in a boundary layer of the fractional Maxwell viscoelastic flow over a vertical plate [42]. By taking the effects of reaction time, Philip n-diffusion flux and thermal diffusivity into account, a modified Fourier law was proposed by Dangui-Mbani et al. [43].

Notice that the CV model can be rewritten into the following form [16]:

$$\mathbf{q}(\mathbf{r},t) = -\frac{k}{\tau}\int_{-\infty}^{t} e^{-\frac{t-t'}{\tau}} \nabla T(\mathbf{r},t')dt' \tag{8}$$

This model has been extended into the following Jeffreys type constitutive law [16]:

$$\mathbf{q}(\mathbf{r},t) = -k_1\nabla T(\mathbf{r},t) - \frac{k_2}{\tau}\int_{-\infty}^{t} e^{-\frac{t-t'}{\tau}} \nabla T(\mathbf{r},t')dt' \tag{9}$$

where k_1 is the effective Fourier conductivity, k_2 is the elastic conductivity. Models (8) and (9) indicate that the heat flux is not only dependent on the temperature gradient at the present time, but also its history. Hence these models reflect the time non-local effect of the nano-scale heat conduction.

Non-local analyses of heat transport are especially interesting in nanosystems, because the mean free paths of phonons with different frequencies may be very different; thus, it is important exploring different kinds of non-local generalizations of the Fourier law, allowing to capture the wide range of phonon mean-free paths (related to non-local effects) in the most efficient phenomenological way. In many models, one takes an average representative mean-free path, but incorporating other features (as for instance the characteristic width of the distribution of mean-free paths) is obviously interesting.

Our proposed constitutive model of the nano-scale heat conduction is based on equation (17), stemming from an analogy with the non-local constitutive model of elasticity proposed in Refs. [44–47]. According to this theory, a stress at a point $\boldsymbol{r}$ in an elastic body is dependent not only on the strain at $\boldsymbol{r}$, but also on strains at all other points of the body. Inspired by this non-local elasticity theory, we attempt to develop a constitutive model accounting for the non-local effect of the nano-scale heat conduction. The microscopic origin of the analogy between the non-local elasticity and the non-local heat conduction may be intuitively understood in the following way. In some elastic models, one must take into account that the system is composed of elastic microscopic fibers of different lengths, such that a simple local description cannot be accurate, as it misses the point of the different contributions of fibers of different lengths. If instead of elastic fibers of different lengths we consider phonons with different mean-free paths, the heat transport response to thermal perturbations will bear some analogies with the elastic response of complex media to mechanical deformations.

2. A non-local constitutive model for nano-scale heat conduction

The CV model (9) accounts for the temporally non-local effect of the heat conduction. However, in Eq. (9) the heat flux and its time derivative at the point $\boldsymbol{r}$ only depends on the temperature gradient at this point. Actually, it is well-recognized that the micro- or nano-scale heat conduction involves not only the diffusive transport, but also the ballistic transport of energy [2,3]. When the size of the heat conduction medium reaches the order of the mean-free path l of the heat carrier, the ballistic transport also plays an important role in the heat transfer. In such a case the heat flux at a point $\boldsymbol{r}$ is not only dependent on the temperature gradient at the point $\boldsymbol{r}$, it also dependent on the temperature gradient at other points in the heat conduction medium, especially the points near the point $\boldsymbol{r}$. Actually, many experimental results have already demonstrated the spatially non-local effect of the nano-scale heat conduction [7–12]. Furthermore, it is reasonable that the influences of the heat carriers on the heat flux at the point $\boldsymbol{r}$ are related to the distance between the location of the heat carriers and the point $\boldsymbol{r}$, normally, the distance is longer, the influence weaker. Based on this viewpoint, for the one-dimensional heat conduction problem the heat flux at the position x should be related to the following integral:

$$\int_0^{L_x} \varphi(x-\bar{x})k\frac{\partial T(\bar{x},t)}{\partial \bar{x}}d\bar{x} \tag{10}$$

where L_x is the length of the heat conduction medium, and $x, \bar{x} \in [0, L_x]$, $\varphi(|x-\bar{x}|)$ is a smooth average kernel and plays the role for designating the weight for the average of the temperature gradient over the heat conduction medium. According to the recent development of the non-local theory of elasticity, we consider the following averaging kernel:

$$\varphi = \frac{1}{2L_{cx}}e^{-\frac{|x|}{L_{cx}}} \tag{11}$$

where L_{cx} is called the characteristic non-local length in the x-direction, and this kernel is called the bi-exponential kernel in the non-local elasticity [46]. The characteristic non-local length depends on the property of materials and should be related to the mean-free path l of the material. According to the definition of the mean-free path which is the average distance travelled by the molecules between collisions, when the heat carrier travels a distance which is equal to or less than the mean-free path, it is quite possible that the heat carrier does not encounter the collision. But when the traveled distance is much longer than the mean-free path, the possibility of the heat carrier to experience collisions becomes higher. Recall that the spatially non-local effect is related to the involvement of the ballistic transport in heat transfer. Therefore, we guess that the characteristic non-local length would be several mean-free paths, that is, $L_{cx} = nl$ where n may vary with different materials. The specific value of n for certain material should be determined by experimental or other methods. The bi-exponential kernel satisfies the following properties [46,47]:

(1) Positivity and symmetry

$$\varphi(x-\bar{x}) = \varphi(\bar{x}-x) \geq 0 \tag{12}$$

(2) Normalization

$$\int_{-\infty}^{+\infty} \varphi(x-\bar{x})d\bar{x} = 1$$

(3) Impulsivity

$$\lim_{L_{cx}\to 0}\int_0^{L_x} \varphi(x-\bar{x})d\bar{x} = \delta(x-\bar{x}) \tag{13}$$

where $\delta(x)$ is the Delta function expressing a unit impulse at the origin. From Eqs. (10) and (12), the integral mean value theorem states that there exists a value $\bar{x}_a \in [0, L_x]$ such that

$$\int_0^{L_x} \varphi(x-\bar{x})k\frac{\partial T(\bar{x},t)}{\partial \bar{x}}d\bar{x} = \frac{k}{2L_{cx}}\frac{\partial T(\bar{x}_a,t)}{\partial \bar{x}_a}\int_0^{L_x} e^{-\frac{|x-\bar{x}|}{L_{cx}}}d\bar{x} \tag{14}$$

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