A MICROSTRUCTURAL APPROACH TO THE BALLISTIC-DIFFUSIVE HEAT TRANSFER

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Summary: The ballistic-diffusive heat model for transient heat conduction problems in low-dimensional structures is presented. Heat carriers are described by space-time distributions within a combined thermodynamic and microstructural diffusive-kinetic approach. From the knowledge of these distributions the resulting equation is then derived and a comparison with other models and its numerical verification are presented.

INTRODUCTION

Over the past decade, micro/nanoscale heat transfer has been the most exciting and active area of research within the heat transfer community. A number of studies have been carried out on the thermal conductivity of thin films and superlattices [1-3]. At low dimensions and at nanolevel scales certain anomalies in macroscopic transport properties such as diffusion and heat conductivity are frequently observed. First, boundary and interface scattering effects in thin films may dominate over volumetric effects such as umklapp and scattering. Secondly, a microstructure or purity of thin films is different from that of a bulk sample. Finally, for some structures, such as superlattices, there are no comparable bulk samples to begin with.
On the nanometer length scale and in ultrafast processes heat pulse is transported both by diffusive and ballistic, or non-local, mechanisms. The paper presents a strategy to investigate the conduction heat transport in thin films in which a ballistic component is superimposed on a regular (diffusive) behaviour. Heat carriers viewed as a collection of randomly moving particles and quasiparticles with hydrodynamic interactions are described by space-time distributions within a combined thermodynamic and diffusive-kinetic approach. Based on the Cattaneo constitutive relation and the additivity of local thermal energy density the hyperbolic ballistic-diffusive heat conduction equation is derived.

MODEL DESCRIPTION

Rigorous treatment of the nanoscale energy transport is becoming increasingly important due to rapid device miniaturization. In turn, many different kinds of particles and/or excitations take part in the energy transport. In our model, a system is considered as being composed of inter-penetrating two subsystems of particles and quasiparticles. A dynamics of the subsystem composed of particles of mass m is derived from an average particle energy $\mathcal{H}_p = \mathcal{H}_p(\mathbf{r}, \mathbf{p})$. The phase space points, with position $\mathbf{r} = \mathbf{r}(t)$ and momentum $\mathbf{p} = \mathbf{p}(t)$, are supposed to move along trajectories defined by Hamiltonian-type equations

$$\frac{d\mathbf{r}(t)}{dt} = \partial_p \mathcal{H}_p(\mathbf{r}, \mathbf{p}), \qquad \frac{d\mathbf{p}(t)}{dt} = -\delta_r \mathcal{H}_p(\mathbf{r}, \mathbf{p}), \tag{1}$$

where $\delta_r \equiv \partial_r - \mathbf{N}_p \partial_p$, $\partial_r \equiv \partial/\partial \mathbf{r}$, $\partial_p \equiv \partial/\partial \mathbf{p}$, and an object $\mathbf{N}_p$ defines a hydrodynamic interaction field in the phase space.
The dynamics of a quasiparticle subsystem is expressed by an average wave frequency (energy) $\mathcal{H}_f(\mathbf{r}, \mathbf{k})$ in terms of the position $\mathbf{r} = \mathbf{r}(t)$ and an average wave vector $\mathbf{k} = \mathbf{k}(t)$ as

$$\frac{d\mathbf{r}(t)}{dt} = \partial_p \mathcal{H}_f(\mathbf{r}, \mathbf{k}), \qquad \frac{d\mathbf{k}(t)}{dt} = -\delta_r \mathcal{H}_f(\mathbf{r}, \mathbf{k}), \tag{2}$$

where $\delta_k \equiv \partial_r - \mathbf{N}_k \partial_k, \partial_k \equiv \partial/\partial \mathbf{k}$.
Eqs (1) and (2) define trajectories in phase spaces along which, respectively, the particle energy $\mathcal{H}_p$ and the wave frequency energy $\mathcal{H}_k$ are vary with time,

$$\frac{d\mathcal{H}_p(\mathbf{p}, \mathbf{r})}{dt} = \mathbf{N}_p \frac{\partial \mathcal{H}_p}{\partial \mathbf{p}} \frac{d\mathbf{r}}{dt}, \qquad \frac{d\mathcal{H}_k(\mathbf{k}, \mathbf{r})}{dt} = \mathbf{N}_k \frac{\partial \mathcal{H}_k}{\partial \mathbf{k}} \frac{d\mathbf{r}}{dt}, \tag{3}$$

where the right hand sides of these equations represent the changes due to collision or interaction processes.
The dynamics of the heat carriers is described by changes with time of a space-time distribution function. A change of particle energy or of wave frequency along a phase space trajectory implies that the particle or quasiparticle interact or collide with other particles or quasiparticles as it traverses such a trajectory. Thus, if $f_p = f_p(\mathbf{p}, \mathbf{r}, t)$ and $f_k = f_k(\mathbf{k}, \mathbf{r}, t)$ define the phase space density of particles and quasiparticles, then changes with time of f_p and f_k along the trajectories (1) and (2) are defined by the microstructure-dependent diffusion equation

$$\frac{\partial f_p(\mathbf{p}, \mathbf{r}, t)}{\partial t} = \frac{\delta}{\delta \mathbf{r}} \left(\boldsymbol{\alpha}(\mathbf{r}, t) \frac{\delta f_p(\mathbf{p}, \mathbf{r}, t)}{\delta \mathbf{r}} \right), \tag{4}$$

where $\boldsymbol{\alpha}$ is the diffusion tensor related to effects of hydrodynamic interactions between particles, and by the relaxation-time Bhatnagar-Gross-Krook (BGK) equation (inferred here from Eq. $(3)_2$)

$$\frac{df_k(\mathbf{k},\mathbf{r},t)}{dt} = -\frac{f_k(\mathbf{k},\mathbf{r},t) - f_{eq}}{\tau_q}, \tag{5}$$

whith the quasiparticle relaxation time τ_q, and f_{eq} the equilibrium distribution of f_k.
Eqs (4) and (5) with the dynamics (1) and (2), and appropriate initial and boundary conditions, constitute the diffusion and collision kinetic equations for particles and quasiparticles.
The essence of the ballistic-diffusive approximation [1] is to decompose the distribution function f at any point of small systems into the diffusive f_p, and the ballistic part f_k. The knowledge of the distribution function $f = f_p + f_k$ enables one to calculate the heat flux as

$$\mathbf{q}(\mathbf{r},t) = \mathbf{q}_p(\mathbf{r},t) + \mathbf{q}_k(\mathbf{r},t), \tag{6}$$

where the diffusive part is averaged over the momentum space, and the ballistic one over the wavevector space.

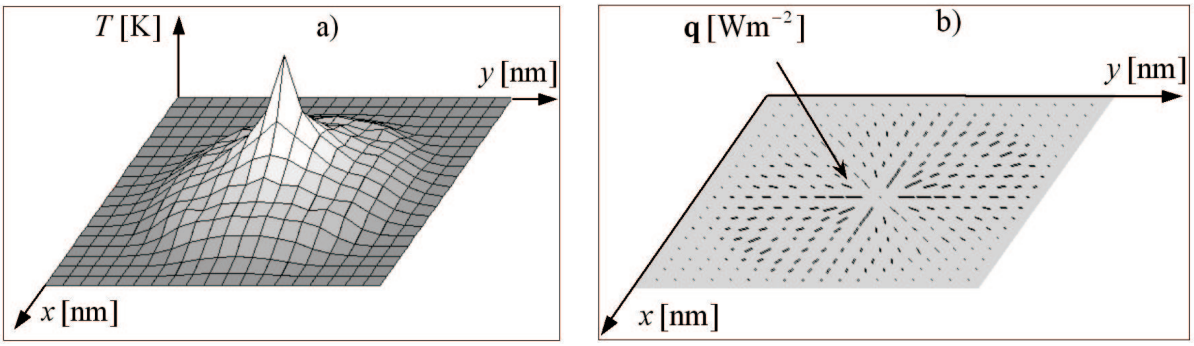

Fig. 1. Heat pulse simulation in thin films: a) temperature profile, b) heat flux vector distribution.

If collisions between particle-particle, particle-quasiparticle, etc., maintain local thermodynamical equilibrium, one can assign a local thermal energy density $u = u(T(\mathbf{r},\mathbf{t}))$ to a particular point of a system. Based on the additive distribution function f, one can introduce two temperatures T_p and T_k such that the rate of internal energy is defined by

$$\frac{\partial u(\mathbf{r},t)}{\partial t} = C\left(\frac{\partial T_p}{\partial t} + \frac{\partial T_k}{\partial t}\right), \tag{7}$$

with $T = T_p + T_k$ considered as the local temperature, and C the heat capacity. Substituting Eqs (6) and (7) into the energy conservation equation, $\partial u/\partial t = -\nabla\cdot\mathbf{q} + \dot{q}_{ex}$, where $\dot{q}_{ex}$ is the heat generation by external heat sources, after eliminating $\mathbf{q}_p$ via the Cattaneo equation and assuming [1]

$$C\left(\tau\frac{\partial^2 T_k}{\partial t^2} + \frac{\partial T_k}{\partial t}\right) + \tau\frac{\partial}{\partial t}\nabla\cdot\mathbf{q}_k = 0,$$

we finally get

$$C\left(\tau\frac{\partial^2 T_p}{\partial t^2} + \frac{\partial T_p}{\partial t}\right) = \nabla(k\nabla T_p) - \nabla\cdot\mathbf{q}_k + \dot{q}_{ex} + \tau\frac{\partial \dot{q}_{ex}}{\partial t}, \tag{8}$$

where k is the thermal conductivity, and τ the relaxation time of $\mathbf{q}_p$.
Our final equation is the same as the equation presented in [1]. The major difference lies in using the microstructure-dependent diffusion and collision-type Boltzmann equations to analyze diffusive-kinetic mechanisms of the heat conduction transport in thin films. In addition, the diffusive-kinetic coupling mechanism can be used in modelling small regions dominated by kinetic effects within a diffusive bulk domain, say, in the vicinity of nanoparticles.

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