International Journal of Thermal Sciences 83 (2014) 56–67

Contents lists available at ScienceDirect

International Journal of Thermal Sciences

journal homepage: www.elsevier.com/locate/ijts

Investigation of highly non-linear dual-phase-lag model in nanoscale solid argon with temperature-dependent properties

Zahra Shomali [a], Abbas Abbassi [b,*]

[a] Department of Physics, Institute for Advanced Studies in Basic Sciences (IASBS), P.O. Box 45195-1159, Zanjan, Iran
[b] Mechanical Engineering Department, Amirkabir University of Technology, 424 Hafez Avenue, P.O. Box 15875-4413, Tehran, Iran

ARTICLE INFO

Article history:
Received 24 July 2013
Received in revised form
30 March 2014
Accepted 22 April 2014
Available online

Keywords:
DPL model
Solid argon
Non-linear behavior
Temperature-dependent properties

ABSTRACT

The one-dimensional non-linear non-Fourier heat conduction within a thin film of solid argon is numerically investigated under the framework of the Dual-Phase-Lagging (DPL) model including the boundary phonon scattering. The thermal properties of the solid argon including the thermal conductivity and sound group velocity are considered to be temperature-dependent, and the results are compared with those obtained from the Molecular-Dynamics simulation for the following cases: (I) constant applied temperature and (II) constant applied heat flux at the left boundary. In addition, each case is studied under two conditions of constant and temperature-dependent volumetric heat capacity. It is concluded that the combination of the DPL model with the mixed-type temperature boundary condition is able to accurately predict the heat flux and temperature distribution obtained from the molecular dynamics simulation. It is also found that using the temperature jump boundary condition along with the DPL model is essential to precisely capture the nanoscale heat transport. The results of our simulation showed that the Knudsen number increases up to 3.86 near right boundary for the temperature dependent volumetric heat capacity.

1. Introduction

In the last decades, by decreasing the size of electronic devices to even less than the phonon-mean-free path of the material, the simulation of micro and nanoscale heat transfer phenomena has attracted great attention. On the other hand, by decreasing the size of the device, results obtained from the classical equations of continuum mechanics gradually deviate from the experimental results. Also, development of high speed laser techniques, in addition to the advancement of nanoscale materials, makes the deviation of transient heat transport from the Fourier's law description become influential where continuum heat diffusion equation is insufficient for describing energy transport at nanoscale. Due to the complexities, difficulties, and obscurities of the atomistic methods, they are developed just for limited fields of heat transfer. Consequently, the development of innovative models to modify the results of classical equations such as Fourier law with less computational cost and more simplicity has attracted a great attention.

The previous researches employed the Fourier's law in the simulation of the thermal systems and neglected the invalidity of Fourier's law at the nanoscale. Cattaneo [1] and Vernotte [2] independently suggested a heat flux model which results in the conventional hyperbolic energy equation considering the heat flux vector evolving after the occurrence of the temperature gradient. The time delay between the occurrence of the temperature gradient and heat flux vector is called the relaxation time.

Recently, the Dual-Phase-Lag model [3–5] as a new modified macroscopic constitutional equation which replaces the Fourier law to simulate the heat transport in some special cases such as micro/nanoscales [6,7], ultra fast laser-pulsed processes [8,9], living tissues [10–14], and Carbon allotropes [15,16] has become the center of attention. The DPL model is capable of demonstrating the new phenomena such as phonon–electron interactions and phonon scattering appearing when the length scale of the problem is reduced down to the mean-free-path of the phonons. This model only deals with the effect of finite relaxation time by applying the heat flux and temperature phase lags where the former is caused by micro structural interactions such as phonon scattering and the latter is the relaxation time due to fast-transient effects of thermal inertia [17].

In a departure from previous studies, we use the DPL model to investigate the transient non-Fourier heat transport in a pure solid

* Corresponding author. Tel.: +98 (21)64543425.
E-mail addresses: z_shomali@iasbs.ac.ir (Z. Shomali), abbassi@aut.ac.ir, abbassi3410@gmail.com (A. Abbassi).

http://dx.doi.org/10.1016/j.ijthermalsci.2014.04.016
1290-0729/

Nomenclature

B	phase-lag ratio
k	heat conduction coefficient (W K^{-1} m^{-1})
v_L	longitudinal sound speed (m s^{-1})
T	temperature (K)
L	size of the film (m)
E_{ss}	steady-state error
k_{BT}	Boltzmann constant (m^2 kg s^{-2} K^{-1})
n	density and direction normal to boundary
t	time (s)
Y	dummy variable (q,T)
C	volumetric heat capacity (J m^{-3} K^{-1})
v	average velocity of sound (m s^{-1})
v_T	transverse sound speed (m s^{-1})
q	heat flux (W m^{-2})
x	direction (m)
r	correlation coefficient
a	argon lattice constant
$\mathbf{r}$	coordinate
t_0	characteristic time (s)

Greek

α	BC coefficient (kg m^{-3})
λ	mean free path of phonons (m)
ω	under-relaxation factor
τ	relaxation time (s)

Superscript

*	non-dimensional condition

Subscript

q	heat flux
L	longitudinal
i	counter
t	gradient temperature
T	transverse

Argon film. In other words, the aim of present work is to test the validity of the DPL model in adequately simulating the transient and steady-state heat transfer in nanoscale systems. Argon film is selected because the energy conduction in such films is dominated purely by phonon transport. Also, due to the availability of a good intermolecular potential for molecular dynamic simulation of argon phonon transport, accurate data close to the experimental values exist to verify our results. In similarity to the work done by Volz et al. [6] and Liu et al. [18], the film is undergone a local temperature change or heat flux at one end which causes the temperature rise used to study the heat conduction in the film. The heat conduction is investigated for two cases of constant temperature and constant heat flux at left boundary, $x = 0.0$. To obtain more realistic results, the temperature-dependent thermal properties of solid argon film including thermal conductivity, sound velocity, and volumetric heat capacity are used. There are some numerical works considering temperature-dependent thermal conductivity [19–23] but to the best of our knowledge the current study is the first research to contemplate the nonlinearity in the DPL model using the more realistic temperature-dependent thermal parameters. Furthermore, the effect of constant heat capacity and temperature-dependent heat capacity of the film for two specified cases are modeled. The governing equations are solved using two coupled first-order fully implicit finite difference scheme with the central discretization of all derivatives. Also, the boundary phonon scattering phenomenon is considered by applying a mixed-type boundary condition.

The details of geometry, boundary condition, mathematical modeling, and numerical approach are introduced in Sections 2–4, respectively. In Sections 5.1–5.4, the temperature and heat flux distributions along the solid argon film are verified using the results of molecular dynamic (MD) simulation for cases I and II with constant volumetric heat capacity. Also, the more realistic condition with the temperature dependent volumetric specific heat is studied.

2. Geometry and boundary conditions

A one-dimensional solid argon thin film is modeled in two cases as discussed below. These cases are considered similar to the case proposed by Volz et al. [6] and Liu et al. [18]. They have used the molecular dynamic techniques on this geometry.

2.1. Case I: constant temperature boundary condition

First, the solid argon thin film with temperature-dependent thermal properties with constant initial temperature is investigated. The left boundary temperature is suddenly increased which results in rearrangement of the temperature distribution in the film. We track down the heat transport in the thin film while the applied temperature over the left boundary is kept constant. This case itself is proceeded for two different systems with: (a) constant volumetric heat capacity (VHC) and (b) temperature-dependent volumetric heat capacity. A system with the constant volume-specific heat capacity, is the one which we adopt to verify our attained results with the available data. Also a step is taken further to make the simulation more realistic.

2.2. Case II: constant heat flux boundary condition

In the second part, we think out of a solid argon film initially kept at monotonous temperature everywhere. A constant energy flux is applied to one end of the film for investigating the temperature and heat flux distribution within the film. While the applied energy flux is preserved constant during the time evolution, as well as the case I, we proceed the simulation for two different types of dependency for volumetric heat capacity.

It should be mentioned that the size of the film, L, is the most effective geometrical parameter of heat conduction phenomenon inside the film. So, this parameter is selected as the characteristic length of the problem. Consequently the value of L controls the magnitude of the Knudsen number, which is the ratio of the phonon-mean-free-path to the characteristic length, $Kn = \lambda/L$. It is important to denote that, due to the temperature reliance of the thermal properties, the phonon-mean-free-path is non-monotonous within the argon film. Therefore, the defined Knudsen number is no longer constant and its value changes as the time or position varies. The size of the argon films in our simulations is taken to be $L = 20$ nm and 10 nm.

3. Mathematical modeling

The single phase-lag model (CV model), indicates that the heat flux vector is the effect which occurs later than the temperature