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Nonlocal heat transfer in two-dimensional Lennard–Jones crystal: Application of the molecular dynamics method

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ABSTRACT

The redistribution of heat between two subsystems in the two-dimensional crystal consisting of particles interacting by means of the Lennard–Jones potential with argon parameters is considered in the frame of molecular dynamics method. Calculations of heat flux, its time derivative and kinetic temperature gradient showed that the characteristic relaxation times of the nonequilibrium flux within the nonlocal Cattaneo model at temperatures $10\,\text{K} < T < 40\,\text{K}$ are very small ($\tau_\nu < 10^{-11}$ s) and, comparable with the time of phonons free path.

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Introduction

The nonequilibrium heat transfer process is described in the conventional approach accepted in the continuum mechanics by means of parabolic type heat equation with inherent paradox of infinite propagation velocity. This fact indicates that this model has limits in its application, and it makes it interesting to investigate the conditions when the local thermodynamic equilibrium and locality principles are used for the description of non-stationary heat transfer based on the Fourier law

$$\vec{q}(\vec{x}, t) = -\lambda(T)\nabla T(\vec{x}, t). \tag{1}$$

becomes unsuitable. Here $T(\vec{x}, t)$ is the temperature, $\vec{q}(\vec{x}, t)$ – heat flux, $\lambda(T)$ – thermal conductivity.

One type of non-local heat and mass transfer models is based on the Cattaneo approach [1,2]. In this model the heat flux relaxation time τ_ν is introduced. Based on this modification the equilibrium and generalized Fourier's law are written as

$$\vec{q}(\vec{x}, t) + \tau_\nu \frac{\partial q(\vec{x}, t)}{\partial t} = -\lambda(T)\nabla T(\vec{x}, t). \tag{2}$$

and the traditional equation of thermal conductivity of parabolic type is converted to a telegraph equation of the hyperbolic type [3] with a limited speed (V_τ) of the disturbances propagation

$$V_\tau = \sqrt{\frac{\chi}{\tau_\nu}}. \tag{3}$$

Here $\chi = \lambda / \rho C_V$ – thermal diffusivity, ρ – density, C_V – thermal capacity.

The heat transfer process was numerically simulated in [3], by means of molecular dynamics (MD) method for the three-dimensional (3D) Lennard–Jones (LJ) system having small number of particles (512), where the thermal conductivity was calculated as

$$\lambda = \frac{\Omega}{3k_B T^2} \int_0^\infty \langle q_l(0) q_l(t) \rangle dt, \tag{4}$$

$$\langle q_l(0) q_l(t) \rangle = \langle q_l(0) q_l(0) \rangle \exp(-t/\tau_\nu). \tag{5}$$

Here Ω – volume, $q_l - q_l$ – l-component of heat flux, τ_ν defines the parameter of the Cattaneo model and it was calculated as

$$\tau_\nu = \frac{\lambda k_B T^2}{\langle q_l(0) q_l(0) \rangle \Omega}. \tag{6}$$

Phonon relaxation time for the system considered was equal to

$$\tau_{ph} = 3\lambda / \rho C_V c_s^2 \tag{7}$$

and had the order 10^{-11} s for temperature interval $60\,\text{K} < T < 130\,\text{K}$. Here c_s – sound velocity.

MD methods are widely used for modeling of thermal processes in the microsystems. Typically the LJ potential is used to describe

the particles interaction, in many cases with the parameters of the inert argon in solid or liquid state [4–7]. Some papers in this field use of the nonlocal Cattaneo model in 3D systems [8–10].

In this paper we want to consider the energy redistribution process between two subsystems with different kinetic temperatures for two-dimensional (2D) model of solid system where identical particles interact by means of the Lennard–Jones potential.

In contrast to [3] the periodic boundary conditions were not used. Actually, the usage of periodic boundary conditions in systems containing a small number of particles can lead to essential nonphysical behavior of thermodynamic parameters. For the sound phonons the critical linear size is defined as [11]

$$R \gg R_c = \frac{c_{char}\hbar}{k_B T} = 10^{-9} \text{ m}, \tag{8}$$

where k_B – the Boltzmann constant, $\hbar$ – the Planck constant, c_{char} defines a characteristic speed of the process (for the acoustic phonon branch is $10^3 - 10^4$ m/s). R_c at $T = 10$ K is of the order of 10^{-9} m. That is valid for argon in the solid state. This evaluation implies that the linear dimension of the system should have a length covering at least 10^2 particles. See also [4,5,8,9] about boundary conditions and new molecular dynamics results for non-local models.

The existence of stochastic behavior in systems with a small number of particles [12,13] has led some researchers to the idea of description of the process of heat transfer based on their molecular dynamic behavior, without using macroscopic equations. The stochastic behavior provides a description of dynamical systems, consisting of relatively small number of particles and it is similar to the behavior of macroscopic systems described in the framework of statistical physics. In this work, the values of the energies of the particles exceed also the limit corresponding to the threshold stochastic behavior of the Lennard–Jones systems.

It should be remarked on that in recent years the number of researches on properties of the two-dimensional and quasi-three-dimensional lattices [14,15] is growing, and one of the goals of our study is the elucidation of the 2D LJ systems thermodynamical properties.

Thus, the special feature of this work is in the study of the heat redistribution in a conservative two-dimensional Lennard–Jones MD system under low temperatures with the parameters of crystal argon.

Numerical calculations of the nonlinear heat equation for the macroscopic continuum model. Thermodynamic parameters 2D and 3D models

Considering the phenomenon of thermal conductivity in macroscopic systems it is necessary to take into account heat transfer parameters depending on the current temperature: thermal conductivity, heat capacity and density of the material. So, this nonlinearity leads to necessity of using the numerical solutions of the standard heat equation

$$\frac{\partial T(x,t)}{\partial t} = \frac{1}{\rho(T) C_V(T)} \frac{\partial}{\partial x}\left[\lambda(T) \frac{\partial T(x,t)}{\partial x}\right]. \tag{9}$$

We realized the corresponding calculations for the Eq. (8) based on the continuum media model to compare them later with the results of molecular dynamic simulations. The one-dimensional nonlinear heat transfer problem was solved for one body, composed on two parts with temperatures T_1 and T_2, respectively.

To solve this task we have to use the values of thermodynamical transfer parameters for 2D LJ systems. It is obvious that thermodynamic parameters of 2D and 3D systems may differ. We will use

expressions for the three-dimensional argon crystal to control and compare.

It was basically for us to apply the values of thermal conductivity, heat capacity and density values obtained from other sources and compare MD results with numerical calculation data.

The heat capacity for argon crystal at low temperatures is very well described by the classical formula [16]

$$C_V^{3D} = 9Nk_B\left(\frac{T}{\Theta^{3D}}\right)^3 \int_0^{\frac{\Theta^{3D}}{T}} \frac{x^4 e^x}{(e^x - 1)^2} dx \tag{10}$$

where Θ^{3D} – the Debye temperature, N – the number of particles, $\Theta^{3D} = \omega_D \frac{\hbar}{k_B}$, ω_D – the Debye frequency.

By analogy with the three-dimensional acoustic phonon system we can write the two-dimensional system as

$$C_V^{2D} = 4Nk_B\left(\frac{T}{\Theta^{2D}}\right)^2 \int_0^{\frac{\Theta^{2D}}{T}} \frac{x^3 e^x}{(e^x - 1)^2} dx. \tag{11}$$

Here and below, the index captures $2D$ applies to the 2D case and index captures $3D$ applies to the 3D one.

Using polynomial approximation we can write the heat capacity in the temperature range $10 \text{ K} < T < 40 \text{ K}$ in J/(kg K) as

$$C_V^{2D} = a_4^{2D} \cdot T^4 + a_3^{2D} \cdot T^3 + a_2^{2D} \cdot T^2 + a_1^{2D} \cdot T + a_0^{2D}, \tag{12}$$

where $a_4^{2D} = 2.985894 \times 10^{-4}, a_3^{2D} = -3.007083 \times 10^{-2}, a_2^{2D} = 0.8692728, a_1^{2D} = -1.75955, a_0^{2D} = -15.27907$, heat capacity in J/(kg K).

The temperature dependence of the 3D system density (ρ^{3D}) [17] may be written approximately as

$$\rho^{3D}(T) = \rho_0(1 - 3.9 10^{-7} T^3). \tag{13}$$

Here ρ_0 – defines the density at zero temperature, which is equal to 1776 kg/m³ for argon. The temperature dependence of the 2D systems density ρ^{2D} may be calculated in the assumption that the linear expansion coefficient is the same for the considered two-dimensional and three-dimensional systems, so

$$\rho^{2D}(T) = \rho_0(1 - 2.6 10^{-7} T^3) \tag{14}$$

In general, we can ignore the temperature density changes, because they are very small.

Average speed of sound in the 3D crystal system (c_s^{3D}) defined usually as

$$c_s^{3D} = (1/c_l^3 + 2/c_t^3)^{-1/3} \tag{15}$$
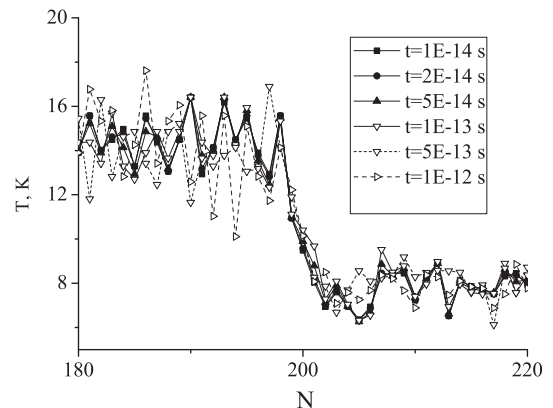
and for the 2D system we write it as

Fig. 1. Column temperature at times $t = 2.5 \times 10^{-12}$, 2.5×10^{-11}, 5×10^{-11}, 7.5×10^{-11} s after connection.