ONE MATHEMATICAL MODEL OF THERMAL CONDUCTIVITY FOR MATERIALS WITH A GRANULAR STRUCTURE

by

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The creation of new materials based on nanotechnology is an important direction of modern materials science development. Materials obtained by using nanotechnology can possess unique physicomechanical and thermophysical properties, allowing to use them effectively in structures exposed to high-intensity thermomechanical effects. An important step of the creation and usage of new materials is the construction of mathematical models to describe the behavior of these materials in a wide range of changes in external influences. One of the possible models for describing the process of thermal conductivity in structurally sensitive materials is proposed in this paper. The model is based on the laws of rational thermodynamics of irreversible processes and models of a continuous medium with internal state parameters. A qualitative study of the constructed model is carried out. A difference scheme is constructed in order to find the solution of the non-stationary heat conduction problem with allowance for the spatial nonlocality effect. The analysis of the solutions is carried out.

Keywords: *non-local effects, curved plate, thermomechanics, non-local deformation, heat conduction, intrinsic state parameter, high-intensity heating.*

Introduction

The development of technology constantly introduces new, higher requirements for existing structural and functional materials. It stimulates the creation of new materials.

Today, properties improvement of such materials is associated with the synthesis of materials from structures that have limited value of properties (for example, extremely strong, refractory, thermostable, *etc*.) Such materials constitute a new class of structural and functional material.

These materials are obtained, mainly, by powder metallurgy, crystallization from an amorphous state, and intense plastic deformation. Features of the structure of such materials (grain size, a significant fraction of the interfaces, porosity, and other structural defects) are determined by the methods of their production and have a significant effect on their physicomechanical and thermophysical properties, which differ significantly from the properties of analogues with coarse-grained or amorphous structure [1-8].

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To date, nano- and sub micro-crystalline structures in the course of intense plastic deformation have been obtained in aluminum, iron, magnesium, tungsten, nickel, titanium, and their alloys [4-9].

Thus, structural and functional materials with micro- and nanostructures have high operational characteristics: strength at a sufficiently high level of plasticity, firmness, high heat capacity, low thermal conductivity, *etc*. Such features make it possible to create fundamentally new designs, devices and instruments with parameters unattainable with the use of traditional materials.

The development of methods for obtaining bulk (solid) billets with uniform structure along the workpiece cross-section, without pores, micro-cracks and other structural defects is an urgent task, the solution of which will allow expanding the use of micro- and nanostructured materials of constructional purpose [4-6].

However, there is a significant gap between the technologies which can create new materials and the possibilities of theoretical prediction of their physical and mechanical properties. Especially it concerns the influence of the local structure of the environment on its macro properties.

The methodology of the continuum does not apply to materials with micro- and nanostructures in pure form. Nevertheless, it is permissible to extend the methods of continuum mechanics that deal with the study of the mechanical behavior of materials at the macro-level to the micro-level. They proved to be very effective [9]. Such propagation of the methods of continuum mechanics is called the method of continuous approximation, and the field of science in which the behavior of materials with micro- and nanostructures is studied using continuous approximation methods is called general mechanics of a continuous medium [9]. The key point in this method is the establishment of a link between the characteristics of the micro (nano) level and the macro-level. Mathematical models of the behavior of such materials must take into account two existing opposing concepts for describing the structure of any solid body – the concept of continuity and discreteness.

In [10-14], thermoelasticity models were introduced using effective variables of temperature and deformation. Based on these models, the temperature and stress fields in a flat layer were analyzed at high-intensity surface heating. In this paper, to obtain the heat equation, we used the approach proposed by Eringen [15]. The approach uses the influence function to describe the effect of non-locality in space, which is reflected in the gradients of the target values.

Mathematical model

To describe the process of transient heat conduction, let us use the model of a medium with internal state parameters. The choice of this approach is explained by the fact that this model allows us to relate the macroscopic behavior of bodies to processes occurring at the molecular and sub molecular levels.

Without taking into account the coupling of the temperature and deformation fields the local formulation of the first law of thermodynamics has the form [16]:

$$\rho T\dot{h} = -\partial q_i / \partial x_i + q_V + \delta \tag{1}$$

where $(^*) = \partial()/\partial t$ and q_i are the projections of the vector of heat flux density on the axis Ox_i of a rectangular co-ordinate system, $i = 1, 2, 3$.

In the case when the characteristic time for changing the external load plays a significant role when developing a thermomechanical model, it is necessary to take into account the

velocity effects both in describing the deformation and in illustrating the process of heat propagation. If the characteristic time of the change in the external load is close in magnitude to the transition time of the thermodynamic system into the new state, then it becomes necessary to consider the change in the internal structural parameters. To consider the local non-equilibrium processes of heat accumulation we introduce the scalar internal state parameter, sometimes called the thermodynamic temperature. The kinetic equation describing the time variation in the linear approximation can take the form [11, 16]:

$$t_T^* \dot{\kappa} + \beta\kappa = \bar{\kappa} \tag{2}$$

where $\bar{\kappa}$ are the functions that determine the equilibrium values of the internal state parameters (of the thermodynamic temperature). Since the thermodynamic temperature, in general, determines the spectrum of frequencies and amplitudes of atomic vibrations on the free surfaces of micro- and nanostructured elements, the coefficient depends on the ratio of the free surface areas and the total area of the element for any small volume element.

Let us define the volume density of free energy in the form of Taylor expansion in a neighborhood of the initial values of the arguments (at the temperature $T = T_0$ of the natural state). Then, for a neighborhood of a point with a radius-vector, x, belonging to the domain, V, occupied by an element of the micro- or nanostructure, we have [16]:

$$\rho A(T,\kappa) = \rho B_1(T) + \rho B_2(T,\kappa) \tag{3}$$

where $A(T_0,T_0) = 0$, $B_1(T_0) = 0$, $B_2(T_0,T_0) = 0$.

In virtue of eq. (3) and relation $h = -\partial A/\partial T$ [16], where A is the mass density of free energy, which is a sufficient condition for the validity of the Clausius-Duhame inequality [11, 16], the energy conservation law (2) can be written in the form:

$$\rho c\dot{T} + \rho c'\dot{\kappa} = -\partial q_i/\partial x_i + q_V + \delta, \quad i = 1, 2, 3 \tag{4}$$

where $c = -T\left(\mathrm{d}^2 B_1/\mathrm{d}T^2 + \partial^2 B_2/\partial T^2\right)$ and $c' = -T\partial^2 B_2/(\partial T\partial\kappa)$ are the specific mass heat capacities that determine the change in free energy proportionally $\dot{T}$ and $\dot{\kappa}$, respectively. The energy dissipation is usually neglected, and we assume that $\delta = 0$ [16].

To obtain the energy conservation law (4) in the form of the heat conduction equation, it is necessary to specify the expression for the equilibrium value of the state parameter $\bar{\kappa}$. Suppose, that $\bar{\kappa} = T(x_i,t)$, that does not contradict with the basic principles of rational thermodynamics of irreversible processes [16].

The relations for the projections of the heat flux density vector, q_i, concerning spatial non-locality are written:

$$q_i = -\lambda_{ij}^{(T)} p_1 \partial T(\mathbf{x},t)/\partial x_j - \lambda_{ij}^{(T)} p_2 \int_V \varphi(|\mathbf{x}'-\mathbf{x}|)\,\partial T(\mathbf{x}',t)/\partial x_j'\,\mathrm{d}x_j' \tag{5}$$

Here $\lambda_{ij}^{(T)}$ are the heat conduction tensor components; $\varphi(|\mathbf{x}'-\mathbf{x}|)$ is the influence function determining spatial non-locality; V is the volume of the non-locality zone, and also:

$$\int_V \varphi(|\mathbf{x}'-\mathbf{x}|)\mathrm{d}\mathbf{x}' = 1 \tag{6}$$

$p_1,\ p_2 \in [0,1]$ are the influence portions of spatial local and non-local effects, $p_1 + p_2 = 1$. The influence function is used in the models offered by Eringen [15] to solve problems in the theory of elasticity and based on the idea that long-range forces that are responsible for non-local deformation of the material at a given point in space are validly described using the distance function $\varphi(|\mathbf{x}'-\mathbf{x}|)$, decreasing with growth $|\mathbf{x}'-\mathbf{x}|$.

Having solved the eq. (2) with respect to κ with the initial conditions $\kappa = T_0$ at $t = 0$, the energy conservation law (4) with provision for the representation (5), can be written in the form of the heat conduction equation:

$$\rho c \frac{\partial T}{\partial t} + \frac{\rho c'}{t_T^*} \int_0^t \exp\left(-\frac{t-t'}{\frac{t_T^*}{\beta}} \right) \frac{\partial T(\mathbf{x},t')}{\partial t'} \mathrm{d}t' = \\ = p_1 \frac{\partial}{\partial x_i} \lambda_{ij}^{(T)} \frac{\partial T(\mathbf{x},t)}{\partial x_j} + p_2 \frac{\partial}{\partial x_i} \lambda_{ij}^{(T)} \int_V \varphi(|\mathbf{x}' - \mathbf{x}|) \frac{\partial T(\mathbf{x}',t)}{\partial x_j'} \mathrm{d}x_j' + q_V \tag{7}$$

The eq. (7) is fundamentally different from the known one, the former allows us to consider the heat conduction process at the macro-level, in view of the delay in heat accumulation, as well as the spatial nonlocality effect.

One-dimensional model

There are comparatively few studies where models of the behavior of a non-local medium are developed with regard to the specific characteristics of the structure. In the present paper, we consider the surface heating problem for a bar in the 1-D setting without taking into account the relation between the temperature and stress fields. Under the assumption that the temperature depends only on time and the co-ordinate directed along the normal inside the body, we write the heat equation as [11, 16]:

$$\rho c \frac{\partial T}{\partial t} = -\frac{\partial q}{\partial x}, \quad x \in (0, L), \quad t > 0 \tag{8}$$

where ρ is a density, c – the heat capacity, and q – the heat flux.

The equation for the heat flux (5) in the one-dimensional case:

$$q(x) = -p_1 \lambda \frac{\partial T}{\partial x} - p_2 \lambda \int_{x-a}^{x+a} \varphi(|x' - x|) \frac{\partial T}{\partial x'} \mathrm{d}x' \tag{9}$$

where a is a radius of the non-locality influence zone filled by the continuum conceived as an aggregate of material particles, linked one another by cohesive bonds (between adjacent particles) and long-range forces.

The influence function is chosen as follows, fig.1, [15, 17, 18]:

$$\varphi(|x' - x|) = \frac{1}{2a} \mathrm{e}^{-\frac{|x'-x|}{a}}, \quad |x' - x| < a \tag{10}$$

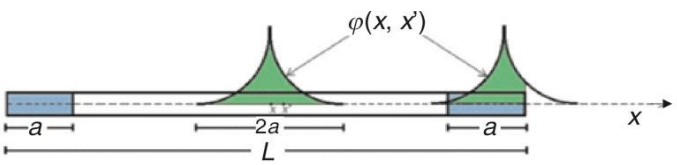

Figure 1. The bar and the influence function

Substituting expression (9) into the eq. (8) we obtain the heat equation, taking into account the non-local effects:

$$\rho c\frac{\partial T}{\partial t}=p_1\lambda\frac{\partial^2 T}{\partial x^2}+p_2\lambda\frac{\partial}{\partial x}\int_{x-a}^{x+a}\varphi(|x'-x|)\frac{\partial T}{\partial x'}\mathrm{d}x',\quad x\in(0,L),\quad t>0 \tag{11}$$

The boundary conditions for the eq. (11) are written in the form:

$$-p_1\lambda\frac{\partial T}{\partial x}-p_2\lambda\int_0^a\varphi(|x'-x|)\frac{\partial T}{\partial x'}\mathrm{d}x'\Bigg|_{x=0}=q_0(t) \tag{12}$$

$$p_1\lambda\frac{\partial T}{\partial x}+p_2\lambda\int_{L-a}^{L}\varphi(|x'-x|)\frac{\partial T}{\partial x'}\mathrm{d}x'\Bigg|_{x=L}=q_1(t) \tag{13}$$

where $q_0(t)$, $q_1(t)$ – the given heat fluxes at the left and right ends of the bar, respectively.

The initial condition is:

$$T(x,0)=T_0=\text{constant} \tag{14}$$

Numerical solution

For the numerical solution of the boundary value problem (11)-(14), a discrete analog was constructed using the integro-interpolation method [19-21].

On the uniform grid, the resulting difference approximation has the form:

$$\rho c\frac{T_i^{j+1}-T_i^{j}}{\tau}h=-p_1q^{(l)}(x)\Big|_{x_i}^{x_{i+1}}-p_2\left[\int_{x-a}^{x+a}\varphi(|x'-x|)q^{(l)}(x')\mathrm{d}x'\right]_{x_i}^{x_{i+1}} \tag{15}$$

The expression for the heat flux at the left boundary of the bar has the form:

$$\begin{aligned}p_1q(0)-p_2\int_0^a\varphi(|x'|)\frac{\partial T}{\partial x'}\mathrm{d}x'=-p_1\frac{\partial T}{\partial x}-p_2\frac{h}{2}\left[c_3q(0)+2c_2\lambda\frac{T_2^{j+1}-T_1^{j+1}}{h}\right]-\\-p_2\frac{h}{2}c_1\lambda\frac{T_3^{j+1}-T_2^{j+1}}{h}=q_0(t)\end{aligned} \tag{16}$$

where c_i is the value of the non-locality influence function at the point x_i. In connection with the symmetry of the function $\varphi(|x'-x|)$, the value of the parameter $j\in\{1,2,3\}$.

Similarly, we arrive at the approximation of the boundary condition on the right boundary of the bar. It should be noted that setting the heat flux in the form (16) leads to the influence of boundary conditions of the second kind not only on the outermost cells, but also on adjacent to them, falling into the segment of the influence of non-locality.

The resulting difference problem leads to a system of linear algebraic equations with a band matrix whose tape width is one more than the number of cells that fall in the segment of the non-locality effect (for the case $2a = 4h$, the matrix is five-diagonal, $2a = 6h$ is a seven-diagonal matrix, *etc.*). The solution of the resulting system of equations can be obtained by any known method.

Analysis of the results

To find a numerical solution, we introduce dimensionless parameters and variables:

$$z=x\sqrt{\frac{\lambda t_0}{\rho c}},\quad \bar{t}=\frac{t}{t_0},\quad \theta=\frac{T-T_0}{T^*},\quad T^*=At_0^m\sqrt{\frac{t_0}{\lambda\rho c}},\quad \bar{a}=a\sqrt{\frac{\rho c}{\lambda t_0}}$$

Calculation for the surface heating when a high-intensity heat flux is given on the left boundary and has the form:

$$q(t) = \frac{m^m \mathrm{e}^{-mt} t^m}{(m-1)!} \tag{17}$$

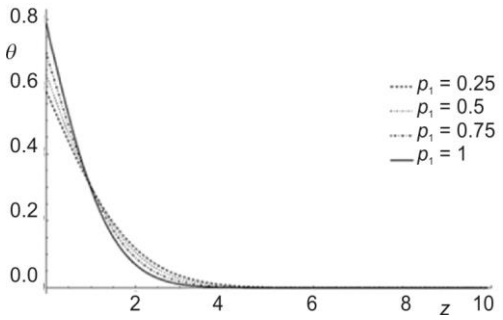

Figure 2. Influence of non-locality parameters on the temperature distribution in the bar

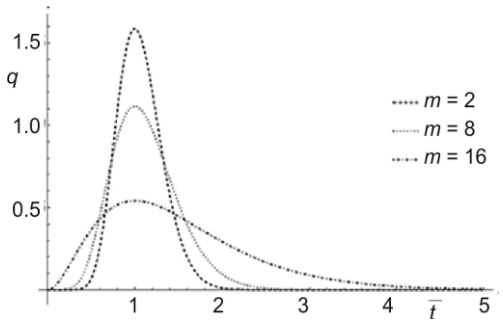

Figure 3. Graphs of the function of high-intensity heat flux at various parameters, *m*

Figure 2 shows the temperature distribution in the bar of length L = 10 at the time $\bar{t} = 2$ for $\bar{a} = 1 = 10h$, $h = 0.1$, $m = 2$ for various values of the parameter p_1. Obviously, with an increase in the share of accounting for nonlocal effects, the temperature at the boundary increases.

Let us consider the effect of the heat flow intensity at different times on the temperature distribution in the bar of length L = 5 with parameters $\bar{a} = 0.2$, $p_1 = 0.5$.

The graphs presented in figs. 3-5 show the temperature distribution in the bar at the instants corresponding to different stages of high-intensity heating. The time moments $\bar{t} = 0.5$, $\bar{t} = 1$, $\bar{t} = 2.5$ correspond to the initial stage, the peak and the final stages of heating, respectively. The graphs show that the solution corresponds to the given boundary conditions.

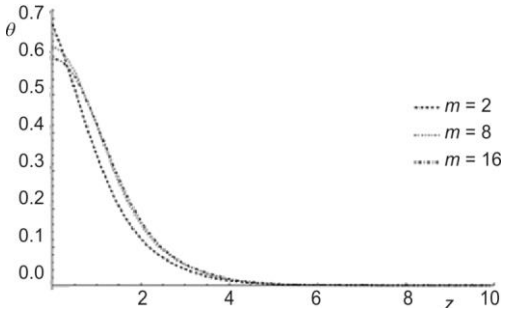

Figure 4. Comparison of the results of calculation of the intensity at various parameters *m* at the time $\bar{t} = 0.5$

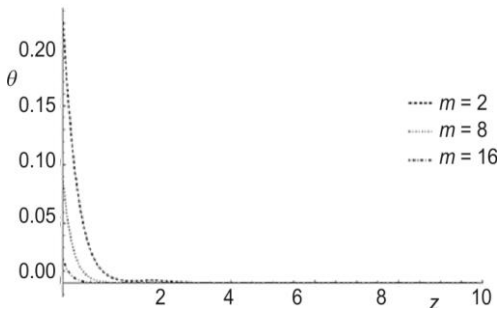

Figure 5. Comparison of the results of calculation of the intensity at various parameters *m* at time $\bar{t} = 2.5$

Results for curvilinear shell

Consider a curvilinear plate of thickness L, mean curvature $\kappa = (1/R_1 + 1/R_2)/2$, where R_1, R_2 – are the principal radii of curvature of the plate surface. The plate is exposed to an external high-intensity pulse. We assume that the thickness of the plate is small in comparison with the radii of curvature, and the external load acts along the normal to the boundary surface. These assumptions make it possible to assume that the temperature field

depends only on time and the co-ordinate x directed along the normal to the interior of the plate [18].

The equation of thermal conductivity, in this case, has the form:

$$\rho c\dot{T} = -\frac{\partial q}{\partial x} - 2\kappa q \tag{18}$$

Consider boundary and initial conditions for eq. (18) in the form (12)-(14). Then the solution can be obtained analogously to the case $\kappa = 0$.

To find a numerical solution, we introduce dimensionless parameters and variables:

$$z = x\sqrt{t_0\lambda/\rho c},\ \ \bar{t} = \frac{t}{t_0},\ \ \theta = \frac{T - T_0}{T^*},\ \ T^* = At_0^m\sqrt{\frac{t_0}{\lambda\rho c}},\ \ q_0(t) = Mt^m\exp(-mt)$$

$$M = \frac{m^m}{(m-1)!},\ \ \bar{\kappa} = \kappa\sqrt{t_0\lambda/\rho c},\ \ \bar{a} = a\sqrt{\rho c/\lambda t_0}$$

Calculation of the temperature field is feasible for a plate thickness $\bar{L} = 10$ at $m = 8$. Figures 6 show the temperature distributions for different values of the share of influence of local effects p_1 and the values of curvature $\bar{\kappa}$. It is seen that the more the influence of nonlocal effects is taken into account (*i. e*., the smaller the value p_1), the lower the temperature.

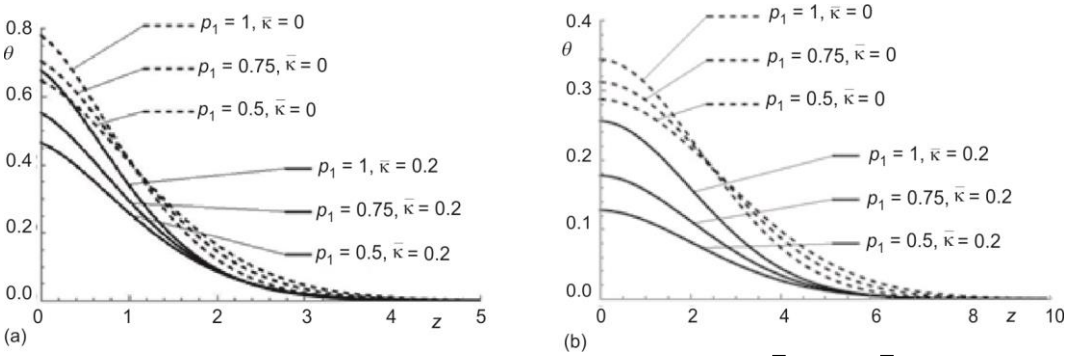

Figure 6. Temperature distributions for various p_1 and $\bar{\kappa}$: (a) $\bar{t} = 2$ (b) $\bar{t} = 5$

Conclusions

The proposed model of thermal conductivity in structurally sensitive materials makes it possible to take into account the spatial non-locality of the medium. The influence of the non-locality and curvature parameters of the plate on the temperature distribution is analyzed. The proposed model of thermal conductivity can be used later in the study of temperature stresses that arise in structural elements under intense thermal action. The value of this model is the ability to predict the properties of new promising materials. It creates the basis for constructing thermodynamic models of the behavior of new structural and functional materials.

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Nomenclature

A – mass density of free energy, [Jkg^{-1}]
c – volumetric heat generation density, [Jkg^{-1}K^{-1}]
h – mass entropy density, [JK^{-1}]
p_1,p_2 – parameters of the contribution of the local and non-local component, [–]
$\mathbf{q}$ – heat flux vector, [Wm^{-2}]
q – 1-D heat flow, [Wm^{-2}]
q_V – volume density of internal heat sources (sinks) power, [Wm^{-3}]
T – temperature, [K]
t – time, [s]
t_T^* – relaxation time of the internal state parameter, [s]
V – scope of influence, [m^3]
x – space co-ordinate, [m]

Greek Symbols

δ – dissipation function, [Wm^{-3}]
κ – mean curvature, [m^{-1}]
ρ – material density, [kgm^{-3}];

Superscripts

l – local vector
nl – non-local vector

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