Mathematical model of the heat transfer process taking into account the consequences of nonlocality in structurally sensitive materials

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Abstract. Creation of new materials based on nanotechnology is an important direction of modern materials science development. Materials obtained using nanotechnology can possess unique physical-mechanical and thermophysical properties, allowing their effective use in structures exposed to high-intensity thermomechanical effects. An important step in creation and use of new materials is the construction of mathematical models to describe the behavior of these materials in a wide range of changes under external effects. The model of heat conduction of structural-sensitive materials is considered with regard to the medium nonlocality effects. The relations of the mathematical model include an integral term describing the spatial nonlocality of the medium. A difference scheme, which makes it possible to obtain a numerical solution of the problem of nonstationary heat conduction with regard to the influence of the medium nonlocality on space, has been developed. The influence of the model parameters on the temperature distributions is analyzed.

1. Introduction
Contemporary structural and functional materials, which are combinations of micro- or nanostructural elements, are often called structurally sensitive materials. An important characteristic of such materials is the qualitative variation in the physical properties compared to massive materials [1–5]. For example, for large fluctuations of physical and mechanical characteristics of micro- or nanostructural elements of the material, the material cannot already be regarded as a simple material, because these characteristics of elements of such a material experience the influence of other surrounding structural elements, i.e., this is the so-called nonlocal medium.

It is well known that the use of methods of continuum mechanics for materials with microstructure is limited by the scale and boundary effects. The direct application of continuum mechanics methods is incorrect for composites modified by nanostructural inclusions [6–10]. Therefore, it is of interest to consider the theory, where, on the one hand, the presence of microstructure is taken into account and, on the other hand, the equations look as the usual equations of continuum mechanics which are generally integrodifferential and which can be solved by methods of continuum mechanics. The method where the concepts of classical continuum mechanics are generalized to media with micro- and nanostructure is called the continuous approximation method [8]. The field of science where the behavior of materials with micro- and nanostructure is studied by continuous approximation methods is sometimes called
continuum mechanics. The main problem in these methods is to determine the relationship between the characteristics of the micro- (nano-) and macrolevels with regard to the effects of spatial nonlocality of the medium.

2. Mathematical model
There are comparatively few studies where models of behavior of a nonlocal medium are developed with regard to specific characteristics of the structure. In the present paper, we consider the surface heating problem for a bar in the one-dimensional 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 coordinate $x$ directed along the normal inside the body, we write the heat equation as $[11, 12]$

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

(1)

where $\rho$ is the density, $c$ is the heat capacity, $q$ is the heat flux.

The model proposed by Eringen is based on the idea that the long-range forces responsible for the nonlocal behavior of the material at a given point $x$ of space can adequately be described using a distance function $\varphi(|x' - x|)$ decreasing with increasing $|x' - x|$ $[10, 13–15]$. The function $\varphi(|x' - x|)$ is called the influence function.

We use this idea to take into account the effect of spatial nonlocality in the model of heat transfer in structure-sensitive materials and assume that the heat flux $q$ satisfies the relation

$$q(x) = -p_1 \lambda \frac{\partial T}{\partial x} - p_2 \lambda \int_{x-a}^{x+a} \varphi(|x' - x|) \frac{\partial T}{\partial x'} dx', \quad x \in (0, L), \quad t > 0,$$

(2)

where $a$ is the radius of the nonlocality influence zone filled by the continuum conceived as an aggregate of material particles linked to one another by cohesive bonds (between adjacent particles) and long range forces, and the parameters $p_1$, $p_2$ are proportions of the influence of local and nonlocal effects, $p_1 + p_2 = 1$.

The influence function is chosen as follows (figure 1) $[10, 16]$: $\varphi(|x' - x|) = \frac{1}{2a} e^{-|x' - x|/a}, \quad |x' - x| < a.$

(3)

Substituting expression (2) into the equation (1), we obtain the heat equation with nonlocal effects taken into account:

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

(4)
The boundary conditions for equation (4) are written in the form:

\[-p_1 \lambda \frac{\partial T}{\partial x} - p_2 \lambda \int_0^a \varphi(|x' - x|) \frac{\partial T}{\partial x'} \, dx' \Big|_{x=0} = q_0(t), \tag{5}\]

\[p_1 \lambda \frac{\partial T}{\partial x} + p_2 \lambda \int_{L-a}^L \varphi(|x' - x|) \frac{\partial T}{\partial x'} \, dx' \Big|_{x=L} = q_1(t), \tag{6}\]

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

The initial condition is \(T(x, 0) = T_0 = \text{const}. \tag{7}\)

3. Numerical solution

To solve problem (4)–(7) numerically, we construct its discrete analogue. We introduce a grid in the domain \(\Omega_T = \{0 \leq x \leq L, 0 \leq t \leq t_0\}\) as follows: \(\omega_h = \{x_i = ih, i = 0, 1, \ldots, n, \ h = L/n\}\) is a uniform grid with step \(h\) on the interval \(0 \leq x \leq L; \ \omega_T = \{t_j = j \tau, j = 0, 1, \ldots, m, \ \tau = t_0/m\}\) is a uniform grid with step \(\tau\) on the interval \(0 \leq t \leq t_0\). Then \(\omega_{hT} = \omega_h \times \omega_T = \{(x_i, t_j), x_i \in \omega_h, t_j \in \omega_T\}\) is a grid in \(\Omega_T\). The temperature value is referred to the cell center. Integrating relation (4) over the cell, we obtain

\[
\rho c \frac{T^{j+1}_i - T^j_i}{\tau} h = p_1 \lambda \frac{\partial T}{\partial x} \bigg|_{x_i}^{x_{i+1}} + p_2 \lambda \left[ \int_{x-a}^{x+a} \varphi(|x' - x|) \frac{\partial T}{\partial x'} \, dx' \right]_{x_i}^{x_{i+1}}. \tag{8}\]

The first term on the right-hand side is responsible for local effects of the medium, and the second term, for nonlocal ones. Let us consider the second term in more detail:

\[
\left[ \int_{x-a}^{x+a} \varphi(|x' - x|) \frac{\partial T}{\partial x'} \, dx' \right]_{x_i}^{x_{i+1}} = \int_{x_{i+1-a}}^{x_{i+1+a}} \varphi(|x' - x_{i+1}|) \frac{\partial T}{\partial x'} \, dx' - \int_{x_{i-a}}^{x_{i+1-a}} \varphi(|x' - x_i|) \frac{\partial T}{\partial x'} \, dx'. \tag{9}\]

We choose a spatial step \(h\) so that an integer number of steps \(h\) fit into the radius \(a\) of nonlocality. In this case, the boundaries of the influence of the nonlocality function fall on the boundaries of the cells.

The integrals in the right-hand side of relation (9) are computed by the quadrature formulas of trapezium. The heat flows are replaced by difference analogs by approximation of the Fourier thermal conductivity law. Then in the case \(a = 2h\), the difference analogue of the heat equation taking into account the nonlocality of the medium has the form

\[
\rho c \frac{T^{j+1}_i - T^j_i}{\tau} h = -p_1 \left( \frac{T^{j+1}_{i+2} - T^{j+1}_{i+1}}{h} - \frac{T^{j+1}_{i+1} - T^{j+1}_i}{h} \right) + \frac{1}{2} p_2 \left[ \lambda \frac{c_1(T^{j+1}_{i+1} - T^{j+1}_{i-1})}{h} + \frac{2c_2(T^{j+1}_{i-1} - T^{j+1}_{i-2})}{h} \right] - \frac{1}{2} p_2 \left[ \lambda \frac{c_1(T^{j+1}_{i+1} - T^{j+1}_{i-1})}{h} + \frac{2c_2(T^{j+1}_{i-1} - T^{j+1}_{i-2})}{h} + \frac{2c_3(T^{j+1}_{i+2} - T^{j+1}_{i+1})}{h} \right] + \frac{1}{2} p_2 \left[ \frac{2c_2(T^{j+1}_{i+1} - T^{j+1}_{i-1})}{h} + \frac{2c_2(T^{j+1}_{i-1} - T^{j+1}_{i-2})}{h} + \frac{2c_3(T^{j+1}_{i+2} - T^{j+1}_{i+1})}{h} \right] - \frac{1}{2} p_2 \left[ \lambda \frac{c_1(T^{j+1}_{i+1} - T^{j+1}_{i-1})}{h} + \lambda \frac{c_1(T^{j+1}_{i+1} - T^{j+1}_{i-1})}{h} \right], \quad i = 4, \ldots, n-5, \quad j = 0, \ldots, m, \tag{10}\]

where \(c_i\) is the value of the nonlocality influence function at the point \(x_i\). Because of the symmetry of the function \(\varphi(|x' - x|)\), the parameter range is \(j \in \{1, 2, 3\}\).
The expression for the heat flux at the left boundary of the bar has the form

\[ p_1 q(0) - p_2 \int_0^a \varphi(|x'|) \frac{\partial T}{\partial x'} \, dx' \]

\[ = -p_1 \frac{\partial T}{\partial x} - p_2 h \frac{1}{2} \left( c_3 q(0) + 2c_2 \lambda \frac{T_{j+1}^j - T_{j+1}^j}{h} + c_1 \lambda \frac{T_{j+1}^{j+1} - T_{j+1}^{j+1}}{h} \right) = q_0(t). \]  

Similarly, we arrive at an approximation of the boundary condition on the right boundary of the bar. It should be noted that setting the heat flux in the form (11) leads to the influence of the boundary conditions of the second kind not only on the outermost cells but also on the cells adjacent to them, thus falling into the segment of the influence of the nonlocality.

The resulting difference problem leads to a system of linear algebraic equations with a band matrix whose tape width is greater by 1 than the number of cells that fall in the segment of the nonlocality effect (in 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.

4. Analysis of the results

We performed calculations for the surface heating in the case where a high-intensity heat flux is given on the left boundary and has the form:

\[ q(t) = \frac{m^m e^{-mt} t^m}{(m-1)!}. \]

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

Fix \( p_1 = 0.5, \ h = 0.1, \) and consider the effect of the nonlocality radius \( a \) on the temperature distribution in the bar at time \( t = 2 \). The graphs in Figure 3 show that the temperature increases with the radius of nonlocality.

Let us consider the influence of the heat flow intensity at different times on the temperature distribution in the bar of length \( L = 5 \) with parameters \( a = 0.2 \) and \( p_1 = 0.5 \).

The graphs presented in Figs. 4–7 show the temperature distribution in the bar at the times corresponding to different stages of high-intensity heating. The times \( t = 0.5, \ t = 1, \ t = 2.5 \) correspond to the initial stage and the peak and final stages of heating, respectively. The graphs show that the solution corresponds to the given boundary conditions.
Figure 4. Graphs of the function of a high-intensity heat flux for different parameters $m$.

Figure 5. Comparison of the results of calculation of the intensity for different parameters $m$ at time $t = 0.5$.

Figure 6. Comparison of the results of calculation of the intensity for different parameters $m$ at time $t = 1$.

Figure 7. Comparison of the results of calculation of the intensity for different parameters $m$ at time $t = 2.5$.

Conclusions
The difference analogue of the one-dimensional heat conduction equation was constructed with regard to the medium nonlocality. The temperature distribution in time was determined and the dependence on radius and parameters of nonlocal nature of the environment was studied. It should be noted that the solution of equation (6) with nonlocality parameter $p_1 = 1$, i.e., where the influence of the nonlocal component is missing, coincides with the solution of the heat equation, where the contribution of the structure nonlocality is not taken into account.

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