Nonlocal dynamic temperature stress simulation

G N Kuvyrkin, I Yu Savelyeva and D A Kuvshinnikova

Department of Applied Mathematics, Bauman Moscow State Technical University, 2nd Baumanskaya St., 5, building 1, Moscow, 105005

E-mail: kuvshinnikovadasha@gmail.com

Abstract. The development of technologies for obtaining consolidated structural materials has increased interest in modelling materials with a heterogeneous structure. For models of such materials, an important factor is the relationship between the characteristics of the micro- (nano-) level and the laws of continuum mechanics at the macro level. The widespread use of modern structure-sensitive materials in extreme conditions is the reason for the urgency of the problem of developing methods of mathematical modelling that allow describing such materials. New nonlinear dynamic problems that arise in this case require a new approach to the study and prediction of the mechanical behavior of such materials under conditions of high-intensity external influences. The paper considers a nonlocal model of dynamic temperature stresses. The model is based on the methods of globalized continuum mechanics. The basic equations of the model are derived from conservation laws. The model of thermomechanical processes in a nonlocal medium includes integro-differential equations with various boundary conditions. Equations describe stress in structural members. Also, the paper proposes an algorithm based on the finite element method to solve the problem. The distributions of temperature stresses in the nonlocal layer of the material are obtained and the influence of the main parameters of nonlocality on the solution of the problem is analyzed.

1. Introduction

The need for non-local thermodynamics in the physical sciences and technology dates to the middle of the last century. Several experimental observations of the temperature field on metal interfaces and changes in the conductivity parameters in the vicinity of thermostated regions show the localization of temperature gradients near the boundaries [1].

In the modern world, similar phenomena are observed in molecular dynamics simulation of heat transfer in nanowires. Modeling shows that the presence of thermostated regions includes phonon-phonon scattering, which changes the conductivity of materials [2, 3].

A rigorous and complete description of the mechanical behavior of real materials is an intricate problem. Usually, to solve specific practical problems, simplifying assumptions about the property of the material and the nature of its behavior are introduced. This replacement of a real substance by an imaginary medium with given properties is the basis for constructing a mathematical model of the material.

Almost all natural and artificially created materials have a complex internal structure, which, moreover, does not remain constant, but changes during external influences and significantly affects the behavior of samples and products made from such materials.
Depending on the type of material and the scale of the study, different models can be used. The higher the scale level of consideration, the less demanding the model is for describing the details of the structure inhomogeneity. At low scale levels, models should describe more details of the structure and at the same time provide a hierarchical description of the connection of low scales with higher ones.

Trends in the development of modern science and technology require the creation of models to describe the behavior of materials with very small features of their structural organization. Such materials are obtained by compaction of nanopowders, deposition on a substrate, crystallization of amorphous alloys, and by means of severe plastic deformation [1]. During creation, such materials acquire structure inhomogeneity, which does not allow them to be described within the framework of classical mechanics of a continuous medium. Due to the peculiarities of their structure, such materials are called "structure-sensitive". The study of structure-sensitive materials becomes possible within the framework of globalized continuous mechanics.

For structure-sensitive materials, the concept of a medium with a microstructure is introduced [2, 3]. It is such a continuous medium, in which each infinitely small "point" carries information about the structure of the material. In comparison with a classical continuous medium, additional forces are most often introduced at the "points" of such complicated media, which contain corrections for the influence of the nearest points.

Currently, models are being developed that can most accurately describe the thermomechanical behavior of structure-sensitive materials under high-intensity external loading. The simplest and most popular is the approach proposed by A.K. Eringen [4–6]. It is based on considering the influence of structure elements on a given point using the nonlocality influence function. This approach is taken in this work as the basis for constructing relationships that allow describing dynamic temperature stresses in structure-sensitive materials.

Earlier, the authors of this work have studied the propagation of heat in nonlocal media [7–11]. Studies have shown that considering the effect of nonlocality in heat propagation is a laborious task. Mathematical models of nonlocal media based on the approach of A.K. Eringen, lead to integro-differential equations that allow describing the thermomechanical state of the medium. An analytical solution to such equations is impossible. In [9], algorithms were proposed for the numerical solution of the problem of heat propagation in a nonlocal medium. The importance of considering non-local effects was shown in [9–11]. In this regard, it became possible to move to a more complex problem - modeling thermoelasticity in nonlocal media. Since this problem was not previously investigated, the authors of this article proposed an approach to building a model and finding numerical solutions. This approach is based in part on previous research.

2. Mathematical model

The heat conduction equation in vector form [11]:

\[ \rho C \frac{\partial T}{\partial t} = -\frac{\partial q_i}{\partial x_i} + q_v^i, \quad i = 1, 3 \]  \hspace{1cm} (1)

where \( \rho \) — is the density of the material; \( c \) — is the heat capacity of the material; \( T(x, t) \) — absolute temperature; \( q_v(x, t) \) — projection of the vector of heat flux density on the axis of the rectangular coordinate system \( O_{x_i} \); \( q_v(x, t) \) — volumetric power density of internal sources (sinks) of heat \( x_i \) — spatial coordinate; \( t \) — time.

In classical models, the heat flow \( q_v(x, t) \) and temperature \( T(x, t) \) are related to the Fourier law of thermal conductivity. For an isotropic and homogeneous body, the law of thermal conductivity has the form [7]:

\[ q_v^0(x, t) = -\lambda_q^0 \frac{\partial T(x, t)}{\partial x_i}, \]  \hspace{1cm} (2)
where $\lambda^{(T)}_{ij}$ — components of the heat conduction tensor.

The effect of nonlocality of the medium is that the physical characteristics of the elements of the structure-sensitive material feel the change in the characteristics of the surrounding elements. The influence of long-range forces is taken into account by modifying the heat flux vector $\vec{q}$:

$$
\vec{q}^{(T)}(x,t) = -p_1 \lambda^{(T)}_{ij} \frac{\partial T(x,t)}{\partial x_j} - p_2 \lambda^{(T)}_{ij} \int_{V} \varphi(|x' - x|) \frac{\partial T(x',t)}{\partial x_j'} dx_j',
$$

where $p_1, p_2$ — the nonlocality (weight) parameters such that $p_1 + p_2 = 1$; $\varphi(|x' - x|)$ — the nonlocal influence function, some normalized positive function in the region $V$.

Substituting equation (3) into the initial equation (1), we obtain the heat conduction equation in vector form, taking into account the nonlocality of the medium:

$$
\rho c \frac{\partial T}{\partial t} = p_1 \frac{\partial}{\partial x_i} \lambda^{(T)}_{ij} \frac{\partial T(x,t)}{\partial x_j} + p_2 \lambda^{(T)}_{ij} \frac{\partial}{\partial x_j} \int_{V} \varphi(|x' - x|) \frac{\partial T(x',t)}{\partial x_j'} dx_j'.
$$

A change in body temperature leads to thermal expansion, which causes the appearance of thermal stresses and deformations inside the solid. The equation describing the arising stresses can be written in the following form [11]:

$$
\sigma_{ij} = C_{ijkl}(\epsilon_{ij}^{(T)} - \epsilon_{ij}^{(T)}),
$$

where $\sigma_{ij}$ — the components of the stress tensor; $C_{ijkl}$ — components of the tensor characterizing the mechanical properties of the body; $\epsilon_{ij}^{(T)}$ — components of the tensor of thermal deformation; $\epsilon_{ij}$ — strain tensor components.

In the case of nonlocality, the components of the deformation tensor are calculated by the formula [11]:

$$
\epsilon_{ij} = p_1 \epsilon_{ij}^{(T)} + p_2 \int_{V} \varphi(|x - x'|) \epsilon_{ij}^{(T)}(x',t) dx'.
$$

Then the equation for determining the stresses (5):

$$
\sigma_{ij} = C_{ijkl} \left( p_1 \epsilon_{ij}^{(T)} + p_2 \int_{V} \varphi(|x - x'|) \epsilon_{ij}^{(T)}(x',t) dx' - \epsilon_{ij}^{(T)} \right).
$$

The corresponding equation for determining the temperature stresses in this case will have the form [7]:

$$
\rho c \frac{\partial T}{\partial t} = -TC_{ijkl} \epsilon_{ij}^{(T)} - \frac{\partial q}{\partial x_i} + q_0,
$$

where $\epsilon_{ij}^{(T)}$ — components of the thermal strain tensor.

Equations (7) — (8) with specified boundary and initial conditions allow describing the thermomechanical behavior of the material.

3. One-dimensional case
Consider the isotropic layer with the heat-insulated side surface. Let the basic physical properties of the material, such as thermal conductivity, heat capacity, and density, be constant.

The thermomechanical load acts along the normal to the boundary surface. The deformation in the direction of this normal is nonzero. Temperature and stresses depend only on time $t$ and coordinates $x$. 

directed along the normal into the body. In this case, the constitutive relations for calculating the temperature stresses are as follows:

\[
\rho c_v \frac{\partial T}{\partial t} = -(3\lambda + 2\mu)T_0 \alpha^{(T)} \dot{\varepsilon} - \frac{\partial q}{\partial x}
\]  
(9)

\[
\sigma = (\lambda + 2\mu) \varepsilon - (3\lambda + 2\mu) \alpha^{(T)} \Delta T
\]  
(10)

where \( c_v \) — the specific mass heat capacity at constant deformation; \( \lambda, \mu \) — Lamé parameters characterizing the elastic properties of the material; \( \alpha^{(T)} \) — temperature coefficient of linear expansion; \( T_0 = \text{const} \) — temperature of the natural state; \( \sigma \) — stress tensor component corresponds to the stress axis \( x \).

To obtain the law of conservation of energy in the form of a heat conduction equation, it is necessary to specify the expression for the vector of the heat flux density \( q(x,t) \) in equation (9). The expression for the heat flux (3) in the one-dimensional case has the form:

\[
q(x,t) = -p_1 \lambda^{(T)} \frac{\partial T(x,t)}{\partial x} - p_2 \lambda^{(T)} \int_{\gamma} \phi(|x' - x|) \frac{\partial T(x',t)}{\partial x'} dx', \quad x \in (0,L), \ t > 0.
\]  
(11)

where \( \lambda^{(T)} \) — coefficient of thermal conductivity.

The constitutive relations of the model of thermomechanical processes in solids can be rewritten in terms of absolute temperature and local deformation. For this, we substitute relations (10) and (11) into (9), and also use the law of conservation of the amount of motion \( \partial \sigma / \partial x = \rho u \) and the Cauchy relation \( \varepsilon = \partial u / \partial x \).

Let \( |T - T_0| / T_0 \ll 1 \), then in the adiabatic process occurring in some control element of the volume, the temperature deviation from the initial one is proportional to the relative change in this volume. The process in question is isentropic. In this case, the parameter of thermoelastic connectivity for many materials will be much less than unity, which makes it possible to neglect the connectivity of the temperature and deformation fields. Let us take the term \( -(3\lambda + 2\mu)T_0 \alpha^{(T)} \dot{\varepsilon} \) in equation (9) equal to 0[12]. In this case, let us turn to the consideration of temperature stresses, which significantly reduces the complexity of the problem being solved.

The equation describing dynamic temperature stresses in a nonlocal layer has the form:

\[
p_1 (\lambda + 2\mu) \frac{\partial^2 \sigma}{\partial x^2} + p_2 (\lambda + 2\mu) \frac{\partial}{\partial x} \left( \lambda^{(T)} \int_{\gamma} \phi(|x' - x|) \frac{\partial \sigma}{\partial x'} dx' \right) = \rho \frac{\partial^2 \sigma}{\partial t^2} + \rho (\lambda + 2\mu) \alpha^{(T)} \frac{\partial^2 T}{\partial t^2}, \quad 0 < x < L, \ 0 < t < T.
\]  
(12)

Introduce dimensionless parameters and variables [6]:

\[
a = \frac{\lambda^{(T)}}{\rho c_v}; \quad z = \frac{x}{\sqrt{at_0}}; \quad \xi = \frac{T - T_0}{T^*}; \quad \xi^* = \frac{At_0^m \sqrt{at_0}}{\lambda}; \quad t_i = \frac{t}{t_0}; \quad Q_1 = \frac{q_1}{At_0^m}; \quad Q_2 = \frac{q_2}{At_0^m};
\]

\[
V_\sigma^2 = \frac{\lambda + 2\mu}{\rho}; \quad \sigma = \frac{\alpha^{(T)}}{(3\lambda + 2\mu) \alpha^{(T)} T^*}; \quad R^2 = \frac{a}{V_\sigma^2 t_0},
\]

where \( a \) — the thermal diffusivity; \( z \) — the dimensionless distance; \( t_0 \) — some point in time; \( t_i \) — the dimensionless time; \( A \) — the dimensional factor; \( Q_1, Q_2 \) — the dimensionless heat flux density; \( R^2 \) —
the dimensionless parameter inversely proportional to the square of the speed of sound, $V_o$, $\theta$ —
dimensionless temperature, $\overline{\sigma}$ — dimensionless stresses.

For simplicity, let's take $a = 1$. Rewrite expressions (9) and (12) taking into account the introduced
dimensionless designations:

$$
\frac{\partial \theta}{\partial t_i} = p_1 \frac{\partial^2 \theta}{\partial z^2} + p_2 \frac{\partial}{\partial z} \left[ \phi(|z'-z|) \frac{\partial \theta}{\partial z'} \right] dz', \ z \in (0, L), t_i > 0.
$$

(13)

$$
p_1 \frac{\partial^2 \overline{\sigma}}{\partial z^2} + p_2 \frac{\partial}{\partial z} \left[ \phi(|z'-z|) \frac{\partial \overline{\sigma}}{\partial z'} \right] dz' = R^2 \left( \frac{\partial^2 \overline{\sigma}}{\partial t_i^2} + \frac{\partial^2 \theta}{\partial t_i^2} \right), \ 0 < z < L, 0 < t_i < \overline{T}.
$$

(14)

The function of influence $\phi$ can be selected in various ways depending on the characteristics of a
specific task. We use the function of influence of nonlocality based on the normal Gaussian distribution
[12]:

$$
\phi(|z'-z|) = \frac{1}{2\pi r} \exp \left( -\frac{|z'-z|^2}{r^2} \right), \ |z'-z| < r,
$$

where $r$ — the radius of influence zone of nonlocality.

Consider a problem with boundary conditions of the second kind for the heat equation (13). For the
equation of motion in stresses (14), we set the boundary conditions of the first kind. Let us write down
the initial and boundary conditions in dimensionless form:

$$
\theta(z, 0) = \theta_o = const, \overline{\sigma}(z, 0) = 0, \overline{\sigma}(z, 0) = 0;

-\frac{\partial \theta(z, t_i)}{\partial z} \bigg|_{z=0} = Q_1(t_i), \quad \frac{\partial \theta(z, t_i)}{\partial z} \bigg|_{z=L} = Q_2(t_i);

\overline{\sigma}(0, t_i) = 0, \overline{\sigma}(L, t_i) = 0.
$$

(15)

Equations (13) - (14) with boundary conditions (15) describe the process of propagation of
temperature and temperature stresses in a nonlocal one-dimensional layer.

4. Numerical solution

A uniform grid with a constant time step $\tau$ is specified. We use the finite element method [13-14] for
equations (13) - (14). We get two systems of linear algebraic equations. The resulting systems of
equations in matrix form:

$$
[C][\theta]^{k+1} + ([K] + [K^{(nl})]) [\theta]^{k} = [F]
$$

(16)

$$
[A_1][\overline{\sigma}]^{k+1} = \{h_2\},
$$

(17)

where

$$
C_{ij} = \int_0^L \phi_i(z)\phi_j(z)dz, \quad K_{ij} = p_1 \int_0^L \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z} dz,
$$

$$
K^{(nl)}_{ij} = p_2 \int_0^L \frac{1}{2r} \int_{z_i-r}^{z_i+r} \exp \left( -\frac{|z'-z|}{r} \right) \frac{\partial N_i(z')}{\partial z'} dz' dz, \quad z_i = z, i = 1, 2, \ldots, N
$$
\[
F_i = Q_i(t)N_i(0) + Q_i(t)N_i(L), \quad A_2 = \tau^2 \left[ K^{(adj)} \right] + \tau \left[ K^{(loc)} \right] + [M];
\]

\[
\{b_2\} = 2[M] \left[ \frac{\sigma}{\tau} \right]^k - [M] \left[ \frac{\sigma}{\tau} \right]^{k-1} - \tau^2 \left\{ f_z \right\}^k, \quad [M] = R^2[C];
\]

\( N_i(z) \) – the basic functions.

Let’s consider in more detail the calculation of a nonlocal matrix coefficients \( K_{ij}^{\text{nonloc}} \). To calculate the integral over the zone of influence of nonlocality, we find the centers of all mesh elements. For each element, we search for the nearest elements relative to its center in the zone of a given radius \( r \). If the center of a neighboring element falls into the zone of influence, then it is taken into account in the calculation. When approximating, the radius is chosen slightly larger than the real radius of the nonlocal influence. Thus, all nodes that fall into the zone of non-local influence participate in the calculation. Note that the distance between the center of the current element and the center of the neighboring element can be calculated in advance for a uniform grid. With fixed centers of the cells, the distances from the current point to the elements that fall into the zone of influence are constant, \( \| z - z' \| = \text{const} \).

Integrals over the zone of influence of nonlocality can be calculated as the sum of integrals over the grid cells included in the zone of influence. For each such grid cell, the value of the nonlocality function will be constant. In this way, the integral can be calculated exactly at a constant spatial step.

Consider, for example, the approximation of the boundary cells for \( r = 3h \). Boundary cells make up the first and last row of the nonclanity matrix \( K_{ij}^{\text{nonloc}} \). For example, consider the right border of the layer.

Figure 1 shows how the basis functions and the first influence function intersect. Since all other basis functions do not intersect the nonlocality influence function, the corresponding terms in formula (17) for \( K_{ij}^{\text{nonloc}} \) (matrix coefficients) are equal to 0.

**Figure 1.** Approximation of basis functions and influence functions at the layer boundary.

When calculating the left-hand side of equation (16), there is a sparse symmetric ribbon-type heat conduction matrix. The width of the matrix tape will be equal to the number of elements that fall into the influence zone. In this regard, the thermal conductivity matrix has fewer zero elements than in the classical formulation, \( p_i = 1 \). The growth of requirements for RAM (random access memory) in a problem with nonlocal effects is quadratic with respect to the number of elements that fall within the radius of nonlocal influence. In the classical setting, the growth of requirements is linear.
5. Results

Structurally sensitive materials can be used as protective coatings for structural elements exposed to high levels of stress. Such influences include high-intensity pulsed heating. The high-intensity pulse heating function can be set as [12, 15]:

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

Consider a layer \( L = 10 \). On the left border, the condition of high-intensity pulsed heating with the intensity parameter \( m = 2 \) (figure 2) is specified. On the right border there is thermal insulation. For stresses, zero boundary conditions of the first kind are specified.

![Figure 2. High-intensity flow functions at the value of the intensity parameter \( m = 2 \).](image)

Consider the influence of nonlocality parameters and material properties of stress in the layer. Figure 3 shows the distributions of temperature stresses in the layer at a time point \( t = 2 \) at different values of the contribution of the local component \( p_1 \). With an increase in the contribution of the nonlocal component (decrease \( p_1 \)), the magnitude of the temperature stresses increases in absolute value at the peak points. The stress peak itself is displaced into the depth of the rod. This effect suggests that structure-sensitive materials absorb thermal effects and can be used as protective coatings against thermal deformations.

Next, consider the effect of the nonlocality diameter on the stress distribution in the layer. Figure 4 shows the distribution of temperature stresses in the layer at a time point \( t = 2 \) at different values of the nonlocality diameter \( 2r \). An increase in the nonlocality diameter "smoothes out" the stress distribution in the layer. In this case, the peak of the values in modulus is shifted into the depth of the layer. This effect is due to the fact that a larger number of values that affect the stresses at a specific point in space fall into the area of influence. Since the number of points falling into the nonlocality region is directly related to the structure of the material, it is determined in the course of a numerical experiment depending on the diameter of the nonlocality region.
Figure 3. Influence of the parameter of the local component contribution on the distribution of temperature stress in the layer.

Figure 4. Influence of the nonlocality diameter on the distribution of temperature stress in the layer.

Figure 5 shows solutions for different parameters $R^2$ in a layer of thickness $L = 10$ at a point in time $t = 2$. With an increase in the parameter $R^2$, the speed of propagation of the stress wave noticeably decreases, but at the same time the amplitude increases. To compare the classical and nonlocal solutions, consider the red and green dashed lines in figure 5. Nonlocal temperature stresses reach their peak faster than the classical ones. By the nature of its propagation, the wave of nonlocal temperature stresses resembles an orange distribution ($R^2 = 10$) with a higher wave propagation speed.
Figure 5. Influence of the speed parameter on the distribution of temperature stresses in the layer.

6. Conclusions
The mathematical model considered in the work makes it possible to simulate thermomechanical processes in a deformable solid under various assumptions regarding the structure of the material. The solution to the dynamic problem of connected thermoelasticity is computationally and practically labor intensive. In the work, simplifying assumptions are made for the transition to the model of temperature stresses. On the basis of the finite element method, a difference analogue of the problem of the propagation of temperature stresses is constructed. Numerical solutions are found for the problem of high-intensity heating of a nonlocal layer. The influence of nonlocality parameters and characteristics of the medium on the obtained solutions is analyzed. A comparison of nonlocal solutions with classical solutions of the problem of the propagation of thermal stresses in an isotropic material is carried out. An important factor in modeling structure-sensitive materials is the influence of non-local effects.

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References
[1] Andrievskii R A and Ragulya A V 2005 Nanostructural Materials (Moscow, Akademiya)
[2] Alymov M I, Zelensky V A 2007 Methods of production and physical and mechanical properties of bulk nanocrystalline materials (Moscow, ELIZ) p 148 (in Russian)
[3] Onami M, Iwashimizu S, Hank K, Shiozawa K and Tanaka K 1987 Introduction to micromechanics (Moscow: Metallurgy) p 280
[4] Eringen A C 2002 Nonlocal continuum field theories (New York-Berlin-Heidelberg: Springer-Verlag) p 393
[5] Eringen A C 2006 Nonlocal continuum mechanics based on distributions (International Journal of Engineering Science 44(3)) pp 141-147
[6] Pisano A A, Fuschi P Closed form solution for a nonlocal elastic bar in tension (England, International journal of Solids and Structures, 40 (2013), 1, pp. 13-23.
[7] Zarubin, V S and Kuvyrkin G N 2008 Mathematical Models of Continuum Mechanics and Electrodynamics (Moscow: The Bauman University Publishing House) p 512
[8] Kuvyrkin G N and Savelyeva I Yu 2019 One mathematical model of heat conduction in nonlocal
[9] Kuvyrkin G N, Savelyeva I Yu, Kuvshinnikova D A 2019 *Non-stationary heat conduction in a curvilinear plate with account for spatial nonlocality* (Springer New York Consultants Bureau, Journal of engineering physics and thermophysics, Vol. 92. N 3) pp 608-613

[10] Kuvyrkin G N, Savelyeva I Yu and Zhuravsky A V 2018 *Numerical Simulation of Vapor-Phase Epitaxy with Allowance for Diffusion Processes* vol 10, issue 3 (Mathematical Models and Computer Simulations) pp 299–307

[11] Zarubin V S, Kuvyrkin G N, Savelyeva I Yu 2013 *Mathematical model of a non-local medium with internal state parameters* (Minsk, Engineering and physical journal, Vol. 86, N 4) pp. 768-773.

[12] Kuvyrkin G N 1993 *Thermomechanics of a deformable solid under high-intensity loading* (Moscow, Bauman Moscow state technical University) p 142 (in Russian)

[13] Zienkiewicz O, Taylor R and Zhu J Z 2013 *The Finite Element Method: Its Basis and Fundamentals. Seventh edition* (Oxford: Butterworth-Heinemann) p 756

[14] Bathe K-J 2014 *Finite Element Procedures. Second edition* (Watertown) p 1065

[15] Kuvyrkin G N, Savelyeva I Y, Kuvshinnikova D A 2018 *Mathematical model of the heat transfer process taking into account the consequences of nonlocality in structurally sensitive materials* (Journal of Physics: Conference Series, 991(1):012050)