

# VARIATIONAL MODELS OF COUPLED GRADIENT THERMOELASTICITY AND THERMAL CONDUCTIVITY

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**Abstract.** We consider generalized variational non-local models of media with fields of defects and show that the methods of continuum mechanics are very effective in modeling connected reversible and irreversible thermomechanical processes. It is postulated that the tensor of free distortions is determined only by the spherical tensor, which is interpreted as a dilatation associated with a change in temperature. A variational model of coupled thermoelasticity and hyperbolic thermal conductivity is under construction. It describes the general case of non-locality, when gradient properties are determined by scale parameters that are responsible for both mechanical and temperature effects. The analysis of boundary value problems is given, the physical interpretation of all model parameters is given through known thermomechanical parameters. We also offer a variation model of irreversible thermodynamic processes, which is based on the principle of L.I. Sedov. In this case, the variation form for the dissipative part of the change in energy is based on the non-integrability condition proposed by the authors.

**Keywords:** non-local models, defective media, free dilatation, variational models, extended thermodynamics, irreversible processes, dissipation model, coupled thermoelasticity and thermal conductivity, physical model, thermo-resistance

## 1. Introduction

It is known that the classical theory becomes insufficient to describe the distribution of heat at low temperatures [1], to understand the thermoelastic properties of small-sized systems [2,3], for the cases of simulating of nanostructured microelectronic components and various thermoelectric devices [4]. On the other hand, it is known that the wave properties of hyperbolic heat transfer can manifest themselves as consequences of scale effects [5,6]. Such problems of heat and mass transfer need to attract more general models of the Maxwell-Cattaneo type [7-10], which are free from contradictions of diffusion type models. Accounting for the effects of connectedness of mechanical and thermal fields should also be carried out using models of extended thermodynamics [11-13]. In work [13] it is noted that models of extended thermodynamics with the wave nature of heat transfer in micro-mechanics of inhomogeneous can be obtained on the basis of generalized non-local theories with two scale parameters.

The approach based on the analysis of the space-time theory of elasticity [14-17] is very effective in building models of extended thermodynamics with allowance for thermoelasticity and thermal conductivity. In recent papers [18-20], closed models of heat transfer using variational approaches have been constructed. Variational models allow us to give correct formulations of the models of coherent thermal conductivity and extended thermodynamics [21].

As it turned out, the space-time elasticity includes traditional thermoelasticity as well as entropy and temperature and allows you to get all the main results of classical thermoelasticity, including relations between thermodynamic coefficients, Duhamel-Neumann hypothesis, equilibrium equations for non-uniformly heated bodies, as well as Fourier and of heat conduction Maxwell-Cattaneo laws.

However, such an approach becomes very laborious for implementation in a space-time continuum, if within it we try to generalize and take into account scale effects, introducing a gradient variant of models. Therefore in this article, the authors try to study the thermomechanics of deformation and coupled heat transfer processes within the framework of the classical consideration.

Size effects in the thermal conductivity and thermoelasticity were investigated in theoretical and experimental studies [22-24]. In [25-27]. It was shown that for inhomogeneous structures, gradient effects and coupled effects and thermal relaxation effects are very important as in assessing the effective thermal conductivity, effective thermomechanical properties as in the study of their dynamic behavior. Recently, in thermomechanics, as well as earlier in the 80s in the mechanics of inhomogeneous media there occurred an interest in the development of generalized applied gradient theories, which allow us to take into account not only strain gradients, but also temperature gradients of a higher order than in classical models. An example of such a continuum thermomechanical theory is the generalized Aifantis theory. In [28], this theory extends to thermomechanical problems; it introduces the concepts of hypertemperature and hyperentropy associated with gradientness. Specially, it is worth to note the interface effects characteristic for heterogeneous materials, especially if the density of the phase boundaries is high. Such effects are associated with thermo-barrier effects at the interfaces [29].

In this article we will try to show that the consistent use of variational methods of mechanics for generalized models of media and the physical model obtained by using Green's formulas, as well as a consistent interpretation of the obtained results allows us to construct a closed energy-consistent mathematical gradient theory of connected thermodynamics of the processes of deformation and heat conduction, i.e. obtain the formulation of governing equations (equations of equilibrium and quasistatic thermoelasticity in the case of quasi stationary processes and equations of motion and Maxwell-Cattaneo dynamic heat conduction in the case of dynamic irreversible processes) and the full spectrum of initial-boundary conditions. At the same time, it is shown that taking into account the gradient of the base models of the media used as the basis for constructing connected models, determines the basic nature of heat transfer which is not local, as is the case in elasticity.

## 2. Variational gradient model with defects field (micro dilatations field)

Let's consider a variant of a model of a medium with defect fields, which, on the one hand, is a gradient, and on the other hand, takes into account the field of defects associated with a free change in volume, micro dilatation. Such a choice of the model is determined by the fact that further we will consider the deformation fields associated with temperature effects. We write the Lagrange functional, which completely defines the physical model and the mathematical model of the media

$$L = A - \frac{1}{2} \iiint_V U_V dV - \frac{1}{2} \iint_F U_F dF, \quad A = \iiint_V P_i^V R_i dV + \iint_F P_i^F R_i dF, \\ 2U_V = G_{ijmn}^{11} R_{i,j} R_{m,n} + K^{11} \theta^1 \theta^1 + 2K^{12} \theta^1 \theta^2 + K^{22} \theta^2 \theta^2 + \\ + C^{11} \theta_{,a}^1 \theta_{,a}^1 + 2C^{12} \theta_{,a}^1 \theta_{,a}^2 + C^{22} \theta_{,a}^2 \theta_{,a}^2, \\ 2U_F = A^{11} \theta^1 \theta^1 + 2A^{12} \theta^1 \theta^2 + A^{22} \theta^2 \theta^2, \quad (1)$$

where  $U_V(R_i, \theta^1, \theta^2)$  is the volume density of the potential energy;  $A$  is the work of external forces;  $P_i^V$  is the forces given in volume  $V$ ; and  $P_i^F$  is the forces given on the surface  $F$  of the body;  $U_F(\theta^1, \theta^2)$  is the density of potential energy of surface interactions, which determines the model of the adhesive properties of the surface of an elastic body;  $R_i, \theta^1, \theta^2$  are the components displacement vector, elastic dilatation and free micro dilatation respectively;  $\theta^1 = R_{i,i}$ ;  $G_{ijmn}^{11} = 2\mu(\delta_{im}\delta_{jn}/2 + \delta_{in}\delta_{jm}/2 - \delta_{ij}\delta_{mn}/3)$  is the tensor of classical elastic moduli associated with shape changing under deformation;  $K^{11}, K^{22}$  are classical bulk modulus and free dilatation bulk modulus respectively;  $K^{12}$  is the bulk modulus which describe the coupled effects;  $C^{11}$  is the gradient modulus;  $C^{12}$  and  $C^{22}$  are coupled gradient modulus and gradient free dilatation modulus;  $A^{pq}, p, q = 1, 2$  are the adhesion properties of the body surface.

The peculiarity of the proposed model is that the gradient nature is determined only by elastic and free dilatation, in other words, the gradient part of the potential energy density  $W_V$  has the following simple form

$$2W_V = C^{11}\theta_{,a}^1\theta_{,a}^1 + 2C^{12}\theta_{,a}^1\theta_{,a}^2 + C^{22}\theta_{,a}^2\theta_{,a}^2.$$

The adhesive model is defined by three constants, one of which  $A^{11}$  determines the surface tension and is similar to the corresponding parameter in the Gurtin-Murdoch model [30], the coefficient  $A^{22}$  determines the "non-classical" adhesion properties associated with free dilatation and  $A^{12}$  characterizes the coupled effects in adhesion.

Constitutive equations for the generalized stresses and generalized kinematic variables (deformations, curvatures of elastic dilatations, free dilatations and their curvatures) in the body volume could be written based on the Green formulas. Cauchy stresses  $\sigma_{ij}^1$ , moments  $m_a^1$ , dislocation stresses  $\sigma_{ij}^2$ , and dislocation moments  $m_a^2$  are the following view:

$$\sigma_{ij}^1 = \frac{\partial U_V}{\partial R_{i,j}} = 2\mu(R_{i,j}/2 + R_{j,i}/2 - R_{r,r}\delta_{ij}/3) + (K^{11}R_{r,r} + K^{12}\theta^2)\delta_{ij}/3, \quad (2)$$

$$\sigma_{ij}^2 = \frac{\partial U_V}{\partial \theta^2} = (K^{12}R_{r,r} + K^{22}\theta^2)\delta_{ij}/3,$$

$$m_a^1 = \frac{\partial U_V}{\partial \theta_{,a}^1} = (C^{11}R_{r,r} + C^{12}\theta^2)_{,a}, \quad m_a^2 = \frac{\partial U_V}{\partial \theta_{,a}^2} = (C^{12}R_{r,r} + C^{22}\theta^2)_{,a}.$$

On the surface of the media, Green equations lead to constitutive equations for the two types of adhesive "forces"  $a^1$  and  $a^2$  that are scalars:

$$a^1 = \frac{\partial U_F}{\partial \theta^1} = A^{11}\theta^1 + A^{12}\theta^2, \quad a^2 = \frac{\partial U_F}{\partial \theta^2} = A^{12}\theta^1 + A^{22}\theta^2. \quad (3)$$

Now we can write the variational equation corresponding to the stationary condition of the Lagrangian (1). Taking into account equations (2), (3) we receive the following variational equation in force terms:

$$\begin{aligned}
\delta L &= \iiint_V P_i^V \delta R_i dV + \iint_F P_i^F \delta R_i dF - \\
&- \iiint_V (\sigma_{ij}^1 \delta R_{i,j} + m_a^1 \delta \theta_{,a}^1 + \sigma^2 \delta \theta^2 + m_a^2 \delta \theta_{,a}^2) dV = \\
&= \iiint_V \{[(\sigma_{ij}^1 - m_{a,a}^1 \delta_{ij})_{,j} + P_i^V] \delta R_i + (m_{a,a}^2 - \sigma^2) \delta \theta^2\} dV + \\
&+ \iint_F \{[P_i^F - (\sigma_{ij}^1 - m_{a,a}^1 \delta_{ij}) n_j] \delta R_i \\
&- (m_a^1 n_a + a^1) \delta R_{r,r} - (m_a^2 n_a + a^2) \delta \theta^2\} dF = 0,
\end{aligned}$$

here  $n_i$  is the unit vector of the normal to the surface of the body.

The last equation can be represented in kinematic variables as follows:

$$\begin{aligned}
\delta L &= \iiint_V \{[\mu \Delta R_i + (\mu + \lambda) R_{j,ji} - C^{11} \Delta R_{r,ri} + \\
&+ K^{12} \theta_i^2 - C^{12} \Delta \theta_i^2 + P_i^V] \delta R_i + \\
&+ (C^{22} \Delta \theta^2 - K^{22} \theta^2 - K^{12} R_{r,r} + C^{12} \Delta R_{r,r}) \delta \theta^2\} dV + \\
&+ \iint_F \{[P_i^F - (\mu(R_{i,j} + R_{j,i}) + \lambda R_{r,r} \delta_{ij} - \\
&- C^{11} \Delta R_{r,r} \delta_{ij} + K^{12} \theta^2 \delta_{ij} - C^{12} \Delta \theta^2 \delta_{ij}) n_j] \delta R_i - \\
&- [(C^{11} R_{j,j} + C^{12} \theta^2)_{,a} n_a + A^{11} R_{j,j} + A^{12} \theta^2] \delta R_{r,r} - \\
&- [(C^{12} R_{j,j} + C^{22} \theta^2)_{,a} n_a + A^{12} R_{j,j} + A^{22} \theta^2] \delta \theta^2\} dF = 0.
\end{aligned} \tag{4}$$

The following assertion holds:

**Theorem 1.** A variational model defined by Lagrangian (1) and by the variational equation (4) in a particular case gives a) a variational formulation of classical thermoelasticity and b) coupled classical thermoelasticity and thermal conductivity.

a) For a given temperature field, the variational model defined by the Lagrangian (1) gives a variational formulation of classical thermoelasticity if the gradient part of the potential energy is zero.

b) With an unknown temperature field, a variational generalized model with the Lagrange functional (1), reduced to the Mindlin model with a field of dilatation defects leads to the formulation of coupled thermoelasticity and thermal conductivity.

**Proof.** We first assume that in the gradient model, (1) the moduli  $C^{pq}$  are equal zero. In this case, the potential energy density  $U_V$  is reduced to the potential energy density for a simplified version of the Mindlin model with a field of defect-dilatations, where the variability of the fields of defects is neglected. Such a model of the defect environment is called conditionally algebraic, because the deficiency can be excluded algebraically from the boundary value problem for displacements, and then determined explicitly by the constructed solution [31]. Thus, we assume that the gradient part of the potential energy is zero:

$$C^{11} \theta_{,a}^1 \theta_{,a}^1 + 2C^{12} \theta_{,a}^1 \theta_{,a}^2 + C^{22} \theta_{,a}^2 \theta_{,a}^2 = 0.$$

In addition, we assume that free dilatation is obviously related to the field of temperature  $T$ , the distribution of which is assumed to be known.

$$D_{ij}^2 = \theta^2 \delta_{ij} = \alpha T \delta_{ij} / 3,$$

where  $\alpha$  is the coefficient of thermal expansion.

The Lagrange functional for the model under consideration (1) takes the following simple form:

$$L = \iiint_V P_i^V R_i dV + \iint_F P_i^F R_i dF - \iiint_V U_V dV,$$

$$2U_V = C_{ijmn}^{11} R_{i,j} R_{m,n} + 2K^{12} R_{i,i} \alpha T + K^{22} \alpha T \alpha T.$$

Accordingly, the variational equality, which determines the mathematical model, can be written in the following form:

$$\delta L = \iiint_V (C_{ijmn}^{11} R_{m,nj} + \tilde{P}_i^V) \delta R_i dV +$$

$$+ \iint_F (\tilde{P}_i^F - C_{ijmn}^{11} n_j R_{m,n}) \delta R_i dF = 0,$$
(5)

where:

$$\tilde{P}_i^V = P_i^V + K^{12} \alpha T_{,i}, \quad \tilde{P}_i^F = P_i^F - K^{12} n_i \alpha T = 0.$$

It is easy to see that the variational equation completely (5) describes the classical thermoelasticity. The first part of the theorem is proved.

We further assume that, as in the models of Mindlin, the gradientity of model is determined only by the presence of the gradient part of the potential energy associated with the gradients of free dilatations and  $C^{22} > 0$  ( $C^{22} \theta_j^2 \theta_j^2 \neq 0$ ,  $D_{ij}^2 = \theta^2 \delta_{ij} = \alpha T \delta_{ij} / 3$ ):

$$L = \iiint_V P_i^V R_i dV + \iint_F P_i^F R_i dF - \iiint_V U_V dV,$$
(6)

$$2U_V = C_{ijmn}^{11} R_{i,j} R_{m,n} + 2K^{12} R_{i,i} \alpha T + K^{22} \alpha T \alpha T + l^2 C^{22} \alpha T_{,k} \alpha T_{,k}.$$

It is easy to see that the Green formulas in this case immediately give the Duhamel Neumann equations for stresses, if we accept that  $K^{12}$  coincides with the bulk modulus of elasticity. The variational equation of the Lagrange principle  $\delta L = 0$  for model (6) is

$$\delta L = \iiint_V [(C_{ijmn}^{11} R_{m,nj} + K^{12} \alpha T_{,i} + P_i^V) \delta R_i +$$

$$+ (l^2 C^{22} \alpha T_{,kk} - K^{22} \alpha T - K^{12} R_{i,i}) \delta(\alpha T)] dV +$$
(7)

$$+ \iint_F [(P_i^F - C_{ijmn}^{11} n_j R_{m,n} - K^{12} \alpha T n_i) \delta R_i - l^2 C^{22} \alpha T_{,k} n_k \delta(\alpha T)] dF = 0.$$

Equation (7) defines a closed boundary problem for the generalized coupled stationary thermo-elasticity-heat conduction, which almost completely coincides with the classical formulation of the coupled problem [32], where coefficient  $l^2 C^{22} = k$  has physical sense of the thermos-conductivity coefficient. The theorem is proved.

We note that, in the resulting generalized variational formulation of a coupled theorem of hermo-elasticity and thermal conductivity, coincides with the classical one if we formally accept in (7) that  $K^{22} = 0$ . However, this condition contradicts the requirement of positive definiteness of potential energy in (1). However, it can be seen that the coupled model (7) actually coincides with the classical formulation, if the coefficient  $K^{22}$  is considered so small compared to  $K^{12}$  and  $(l^2 C^{22})$  so that the second term in the generalized heat equation can be neglected (the second Euler equation in (7)) compared to the other two terms. It can be shown formally that for any boundary problem it is always possible to choose such a value of  $K^{22} > 0$  that the solution of the coupled model (7) coincides with the solution of the classical coupled problem with any predetermined accuracy.

### 3. Generalized mathematical model of coupled thermoelasticity and thermal conductivity. Analysis of the mathematical formulation

By equating to zero the first variation of (4) with respect to admissible kinematic fields  $\delta R_i$  and  $\delta \theta^2$ , we obtain the following equilibrium equations:

$$\mu \Delta R_i + (\mu + \lambda) R_{j,ji} - C^{11} \Delta R_{r,ri} + K^{12} \theta_i^2 - C^{12} \Delta \theta_i^2 + P_i^V = 0, \quad (8)$$

$$C^{22} \Delta \theta^2 - K^{22} \theta^2 - K^{12} R_{r,r} + C^{12} \Delta R_{r,r} = 0. \quad (9)$$

The interpretation of equilibrium equations (8), (see also (4)) is quite obvious. The system of equations (8) should be considered as a system of three-dimensional thermoelasticity equilibrium equations, written in displacements, where the terms containing  $\theta_i^2$  determine the volume change associated with the temperature field. The scalar equilibrium equation (9) remains to be interpreted as the "heat conduction" equation. So, the system of equations (8), (9) determines the system of equations of coupled thermoelasticity-thermal conductivity.

The following natural/essential boundary conditions are derived by such variational procedure. Accordingly, the terms in the surface integral (4) give three pairs of alternative almost "classical" boundary conditions for the generalized thermoelasticity:

$$\iint_F [P_i^F - (\mu(R_{i,j} + R_{j,i}) + \lambda R_{r,r} \delta_{ij} - C^{11} \Delta R_{r,r} \delta_{ij} + K^{12} \theta^2 \delta_{ij} - C^{12} \Delta \theta^2 \delta_{ij}) n_j] \delta R_i dF = 0 \quad (10)$$

and a pair of scalar boundary conditions due to gradient-dilatation theory

$$\iint_F [(C^{11} R_{r,r} + C^{12} \theta^2)_{,a} n_a + A^{11} \theta^1 + A^{12} \theta^2] \delta R_{r,r} dF = 0. \quad (11)$$

At last, a pair of scalar boundary conditions for static temperature distribution problem have view:

$$\iint_F [(C^{12} R_{r,r} + C^{22} \theta^2)_{,a} n_a + A^{12} \theta^1 + A^{22} \theta^2] \delta \theta^2 dF = 0 \quad (12)$$

Equations (8) if we take  $K^{12} = C^{12} = 0$  are the equilibrium equations for a medium with a gradient of restricted dilatation, which, in the case of an additional condition  $C^{11} = 0$  are reduced to the equilibrium equations of the classical theory of elasticity. Note that in the case of taking into account the adhesion and smooth surface of the body, classical boundary conditions in (1) are modified by the term  $\iint_F A^{11} \theta^1 \delta R_{r,r} dF$  in (11) and take the form

$$\iint_F [P_i^F - (\mu(R_{i,j} + R_{j,i}) + \lambda R_{r,r} \delta_{ij} - A^{11} R_{r,rk} \delta_{ik}^*) n_j] \delta R_i dF = 0.$$

It is easy to show that these boundary conditions take into account the surface tension and the resistance of the surface to bending.

*Remark.* We note that the presented variational equation (7), where the same type of boundary conditions are set on the all body surface, does not at all limit the class of possible boundary value problems. Indeed, using the variational principles of mechanics, boundary value problems can always be reduced formally to the first main problem, when external forces are given on the all surface of the body. This is due to the fact that the kinematic connections on the surface of the body can be introduced as the work of reactive force factors on the introduced kinematic connections on the part of the surface where generalized displacements are specified.

As an example, we consider the variational equation of the classical theory of elasticity, when force factors are given on the all surface:

$$\iiint_V [G_{ijmn}R_{m,nj} + K^{11}R_{j,ji} + P_i^V] \delta R_i dV + \iint_F [P_i^F - (G_{ijmn}R_{m,n} + K^{11}R_{m,m} \delta_{ij} / 3)n_j] \delta R_i dF = 0.$$

Assume that external surface loads are given a part of the surface  $F_\sigma$ , and displacements are given on its other part  $F_R$ ,  $F = F_\sigma \cup F_R$ . We take into account the kinematic relations on a part of the surface  $F_R$  using the method of Lagrange multipliers and introducing indefinite Lagrange multipliers  $p_i$ . As a result, the variation of the extended Lagrange functional is written as:

$$\begin{aligned} & \iiint_V [G_{ijmn}R_{m,nj} + K^{11}R_{j,ji} + P_i^V] \delta R_i dV + \\ & + \iint_{F_\sigma} [P_i^F - (G_{ijmn}R_{m,n} + K^{11}R_{m,m} \delta_{ij} / 3)n_j] \delta R_i dF + \\ & + \iint_{F_R} [p_i - (G_{ijmn}R_{m,n} + K^{11}R_{m,m} \delta_{ij} / 3)n_j] \delta R_i + (R_i - R_i^F) \delta p_i] dF = 0. \end{aligned}$$

The received variational equation defines a boundary value problem in the volume  $V$ , bounded by the surface  $F = F_\sigma \cup F_R$ . Assume that a solution of the formulated above the boundary problem can be found in displacements. Then, computing the Lagrange multiplier  $p_i$  from the equation

$$p_i = (G_{ijmn}R_{m,n} + K^{11}R_{m,m} \delta_{ij} / 3)n_j$$

we formally can introduce the formulation of the first boundary problem instead the initial problem with mixed boundary conditions.

The statement is proved. The above reasoning formally extends to the variational formulation for a generalized model of media

Equations (8), (9) are the governing equations of the generalized coupled stationary problem of thermoelasticity and heat conduction. Formally, volumetric deformation  $\theta^1$  can be excluded from these equations. As a result, it is possible to write the governing equation of generalized stationary heat conduction through free dilatation  $\theta^2$  and, therefore, in terms of temperature. This equation obviously generalizes the equation of stationary heat conduction, which follows from the variational formulation (7).

Under the same assumptions that were introduced earlier and under the condition that there are no volume forces and heat sources, in the case under consideration we arrive at the gradient equation of stationary heat conduction

$$k[\Delta T - l_T^2 \Delta \Delta T] = 0, \tag{13}$$

where

$$\begin{aligned} k &= (l_1^2 + l_2^2), \quad l_T^2 = l_1^2 l_2^2 / (l_1^2 + l_2^2), \\ \frac{[C^{11} - 2C^{12}(K^{12} / K^{22}) + C^{22}(2\mu + \lambda) / K^{22}]}{[2\mu + \lambda - (K^{12} K^{12}) / K^{22}]} &= l_1^2 + l_2^2, \\ \frac{(C^{22} / K^{22})(C^{11} - C^{12} C^{12} / C^{22})}{[2\mu + \lambda - (K^{12} K^{12}) / K^{22}]} &= l_1^2 l_2^2. \end{aligned}$$

Here  $l_T$  is the scale temperature parameter, which is expressed through the scale characteristics of the gradient-dilatation model  $l_1$ ,  $l_2$  and are connected with modules of the generalized model (4).

For gradient thermal conductivity with equation (13), we can formally write the variational formulation of the functional which is determined by the following expressions for the density of "potential" energy in the volume and on the surface:

$$2U_V = k_V l_T^2 \Delta T \Delta T + k T_{,k} T_{,k}, \quad 2U_F = aTT + 2bT(T_{,i}n_i) + R_s(T_{,i}n_i)(T_{,j}n_j). \quad (14)$$

The surface energy density  $U_F$  in (14) corresponds to the adhesion model introduced in the general model, with the last term appearing due to the fact that when we exclude from the equations (8), (9) the volume deformation, it is established that  $\theta^1$  is proportional not only to  $\theta^2$ , but also to  $\Delta\theta^2$ . The role of the coefficient  $R_s$  is extremely interesting, because as will be shown later, this coefficient reflects the property of thermal resistance of the contact boundaries of various phases in contact problems of heat transfer for inhomogeneous structures.

A variation formulation that takes into account the surface effects (14), introduced in the general formulation and written in variations, is given below.

$$\begin{aligned} & \iiint_V k (l_T^2 \Delta \Delta T - \Delta T) \delta T dV + \\ & + \iint_F [(-\tilde{P}^F - k l_T^2 \Delta T_{,i}n_i + k T_{,i}n_i - aT - bT_{,i}n_i) \delta T + \\ & + (k l_T^2 \Delta T - bT - R_s T_{,i}n_i) \delta(T_{,j}n_j)] dF = 0. \end{aligned} \quad (15)$$

The coefficients  $a$ ,  $b$  in the integral over the surface (15), i.e. in classical and non-classical boundary conditions describe the generalized effects of heat transfer.

Note that, on the one hand, variational equality (15) is a consequence of the general variational formulation formulated for the Lagrange functional (7) in terms of generalized displacements for a gradient medium with fields of defects – dilations. Indeed, equation (13) was obtained by excluding volumetric strain  $\theta^1$  from equations (8), (9), and is a consequence of the Euler equations (8), (9) in variational equation (7).

On the other hand, the formulated variational equality (15), written in terms of temperature only, can be considered as a variational equation written for the Gibbs potential, taking into account that temperature can be interpreted as generalized stresses in the extended thermodynamics [20]. We believe that variational equation (15) may be useful for engineering applications.

#### 4. Variational model of dynamic coupled thermoelasticity and thermal conductivity

Irreversible processes in continuum mechanics are considered. We use a variational Sedov's principle, in according to which, for irreversible processes, only a variational form can be written, which in general case is non-integrable

$$\delta L + \overline{\delta D_1} = 0, \quad (16)$$

where  $L = A + K - U$  is dynamic Lagrangian,  $A$ ,  $K$ ,  $U$  are the work of given forces in the volume and on the surface of the body, the kinetic energy and potential energy, respectively;  $\overline{\delta D_1}$  is nonintegrable variational form, which describes the dissipative channels.

So, in the common case it can be divided into integrable and nonintegrable parts. The integrable part corresponds to reversible processes and can be represented as the variation of the possible work, kinetic and potential energy. For linear media, potential energy is a quadratic form of its arguments.

In the work [33], algorithm of definition of nonintegrable variational form was proposed when the kinematic variables are known.



Assume that the dissipation process is associated only with thermal processes, i.e. the dissipation channel  $\overline{\delta D_1}$  is determined by the kinematic parameters  $\theta^2$  and  $\dot{\theta}^2$  where  $\dot{\theta}^2 = \partial\theta^2 / \partial t$ , and  $t$  is the physical time of the process. The simplest is the following model of dissipation [33]:

$$\begin{aligned} \overline{\delta D_1} &= \frac{1}{2} \int \left[ \iiint_V D(\theta^2 \delta\dot{\theta}^2 - \dot{\theta}^2 \delta\theta^2) dV \right] dt = \\ &= \int \left[ \iiint_V (-D\dot{\theta}^2 \delta\theta^2) dV \right] dt + \left. \iiint_V \frac{1}{2} D\theta^2 \delta\theta^2 dV \right|_0^t. \end{aligned} \quad (17)$$

Here  $D$  is the physical constant that describes the dissipation properties of the thermodynamic process of the deformation.

To implement Sedov's principle, we write the expressions of the volume density of potential energy and the density of kinetic energy:

$$\begin{aligned} 2U_V &= 2\mu\gamma_{ij}\gamma_{ij} + \\ &+ K^{11}\theta^1\theta^1 + 2K^{12}\theta^1\theta^2 + K^{22}\theta^2\theta^2 + \\ &+ C^{11}\theta_{,i}^1\theta_{,i}^1 + 2C^{12}\theta_{,i}^1\theta_{,i}^2 + C^{22}\theta_{,i}^2\theta_{,i}^2, \end{aligned} \quad (18)$$

$$\begin{aligned} 2K_V &= \rho\dot{R}_i\dot{R}_i + \\ &+ \rho^{11}\dot{R}_{i,i}\dot{R}_{j,j} + 2\rho^{12}\dot{R}_{i,i}\dot{\theta}^2 + \rho^{22}\dot{\theta}^2\dot{\theta}^2, \end{aligned} \quad (19)$$

here  $\rho$  is the classical density,  $\rho^{11}$  is the gradient density, the measure of inertia of volume change,  $\rho^{22}$  and  $\rho^{12}$  are the measure of inertia of free dilation and, accordingly, the measure of inertia of coupled dynamic processes of free and constrained dilatation.

As a result, taking into account the relations (16), (17) and (18), (19) we can find the variational equation of Sedov:

$$\begin{aligned} \delta(A + K - U) + \overline{\delta D_1} &= \\ &= \int \left[ \iiint_V P_i^V \delta R_i dV + \iint_F P_i^F \delta R_i dF \right] dt + \\ &+ \int \left\{ \iiint_V [\rho^{11}\dot{R}_i\delta\dot{u}_i + (\rho^{11}\dot{R}_{j,j} + \rho^{12}\dot{\theta}^2)\delta\dot{R}_{i,i} + (\rho^{21}\dot{R}_{j,j} + \rho^{22}\dot{\theta}^2)\delta\dot{\theta}^2] dV \right\} dt \\ &+ \int \left\{ \iiint_V [-(G_{ijmn}R_{m,n} + K^{11}\theta^1\delta_{ij} + K^{12}\theta^2\delta_{ij})\delta R_{i,j} - (C^{11}u_{m,mk} + C^{12}\theta_{,k}^2)\delta R_{i,ik} - \right. \\ &\left. -(K^{21}R_{i,i} + K^{22}\theta^2)\delta\theta^2 - (C^{21}R_{j,ji} + C^{22}\theta_{,i}^2)\delta\theta_{,i}^2] dV \right\} dt + \\ &+ \int \left[ \iiint_V (-D\dot{\theta}^2\delta\theta^2) dV \right] dt + \left. \iiint_V \frac{1}{2} D\theta^2\delta\theta^2 dV \right|_0^t. \end{aligned}$$

We transform this expression using integration by parts. Finally, we obtain the following variational equation:

$$\begin{aligned}
& \int \left\{ \iiint_V [G_{ijmn} R_{m,nj} + K^{11} \theta_{,i}^1 + K^{12} \theta_{,i}^2 - (C^{11} \Delta R_{m,mi} + C^{21} \Delta \theta_{,i}^2) + \right. \\
& + (-\rho \ddot{R}_i + \rho^{11} \ddot{R}_{j,ji} + \rho^{12} \ddot{\theta}_{,i}^2) + P_i^V ] \delta R_i dV \Big\} dt + \\
& + \int \left\{ \iiint_V [-K^{21} R_{i,i} - K^{22} \theta^2 + (C^{21} \Delta R_{i,i} + C^{22} \Delta \theta^2) - D \dot{\theta}^2 + \right. \\
& + (-\rho^{21} \ddot{R}_{j,j} - \rho^{22} \ddot{\theta}^2)] \delta \theta^2 dV \Big\} dt + \\
& + \int \left\{ \iint_F [P_i^F - (G_{ijmn} R_{m,n} + K^{11} \theta^1 \delta_{ij} + K^{12} \theta^2 \delta_{ij} - \right. \\
& - (C^{11} \Delta R_{k,k} + C^{12} \Delta \theta^2 + \rho^{11} \ddot{R}_{k,k} + \rho^{12} \ddot{\theta}^2) \delta_{ij}) n_j ] \delta R_i dF \Big\} dt - \\
& - \int \left\{ \iint_F [(C^{11} R_{m,mk} + C^{12} \theta_{,k}^2) n_k \delta R_{i,i} + (C^{21} R_{j,ji} + C^{22} \theta_{,i}^2) n_i \delta \theta^2] dF \right\} dt - \\
& + \left. \iiint_V (\rho \dot{R}_i - \rho^{11} \dot{R}_{j,ji} - \rho^{12} \dot{\theta}_{,i}^2) \delta u_i dV \right|_0^t + \left. \iint_F (\rho^{11} \dot{R}_{j,j} + \rho^{12} \dot{\theta}^2) n_i \delta R_i dF \right|_0^t + \\
& + \left. \iiint_V (\rho^{21} \dot{R}_{j,j} + \rho^{22} \dot{\theta}^2 + D \theta^2 / 2) \delta \theta^2 dV \right|_0^t = 0. \tag{20}
\end{aligned}$$

The following statement takes the place.

**Theorem 2.** Equation (20) gives a closed, consistent mathematical model of the deformation process under consideration, including the physical model, the equations of motion of the considered gradient medium under thermoelastic loading and connectivity, the generalized equation of gradient thermal conductivity (and the Maxwell- Cattaneo equation in particular), the initial boundary value problem generally.

**Proof.** Indeed, the equations of motion of a dynamic gradient thermoelasticity immediately follow from the variational equation (20) as the Euler equations with a variational statement. The expression in equation (20) for the variation of displacements  $\delta u_i$  is a vector equation of motion of the medium, i.e. generalized dynamic thermoelasticity equation:

$$G_{ijmn} R_{m,nj} + K^{11} R_{m,mi} - C^{11} \Delta R_{m,mi} - \rho \ddot{R}_i + \rho^{11} \ddot{R}_{m,mi} + K^{12} \theta_{,i}^2 - C^{21} \Delta \theta_{,i}^2 + \rho^{12} \ddot{\theta}_{,i}^2 + P_i^V = 0. \tag{21}$$

Similarly, equating to zero the expression for the variation of free dilatation  $\delta \theta^2$  we will obtain as the Euler equation, the dynamic equation of the gradient thermal conductivity:

$$-K^{21} R_{i,i} + C^{21} \Delta R_{i,i} - \rho^{21} \ddot{R}_{j,j} - K^{22} \theta^2 + C^{22} \Delta \theta^2 - D \dot{\theta}^2 - \rho^{22} \ddot{\theta}^2 = 0. \tag{22}$$

Let us consider the surface integrals in (20) and show that they define the full set of boundary conditions. Indeed, these equations include all set pairs of alternative conditions for the considered gradient coupled dissipative problem, which can be written in the form of variational equality:

$$\begin{aligned}
& \int \left\{ \iint_F [P_i^F - (G_{ijmn} R_{m,n} + K^{11} \theta^1 \delta_{ij} + K^{12} \theta^2 \delta_{ij} - \right. \\
& - (C^{11} \Delta R_{k,k} + C^{12} \Delta \theta^2 + \rho^{11} \ddot{R}_{k,k} + \rho^{12} \ddot{\theta}^2) \delta_{ij}) n_j ] \delta R_i dF \Big\} dt - \\
& - \int \left\{ \iint_F (C^{11} R_{m,mk} + C^{12} \theta_{,k}^2) n_k \delta R_{i,i} dF \right\} dt - \\
& - \int \left\{ \iint_F (C^{21} R_{j,ji} + C^{22} \theta_{,i}^2) n_i \delta \theta^2 dF \right\} dt = 0. \tag{23}
\end{aligned}$$

The last three terms in (20) contain pairs of conditions that define the spectrum of the initial conditions:

$$\begin{aligned} & \iiint_V (\rho \dot{R}_i - \rho^{11} \dot{R}_{j,ji} - \rho^{12} \dot{\theta}_i^2) \delta R_i dV \Big|_0^t + \iint_F (\rho^{11} \dot{R}_{j,j} + \rho^{12} \dot{\theta}^2) n_i \delta R_i dF \Big|_0^t + \\ & + \iiint_V (\rho^{21} \dot{R}_{j,j} + \rho^{22} \dot{\theta}^2 + D\theta^2 / 2) \delta \theta^2 dV \Big|_0^t = 0. \end{aligned} \quad (24)$$

Let us consider the physical relations. The constitutive relations are found using the Green formulas and (18):

$$p = \frac{\partial U_V}{\partial \theta^1} = K^{11} R_{k,k} + K^{12} \theta^2, \quad (25)$$

$$T = \frac{\partial U_V}{\partial \theta^2} = K^{21} R_{k,k} + K^{22} \theta^2. \quad (26)$$

As a result, the Duhamel-Neumann law immediately follows from the constitutive equations of the model (see (25), (26)). In addition, equality (26) shows that temperature along with pressure has a meaning of generalized stresses in the model under consideration, which fully corresponds to the model of extended thermodynamics considered in [33].

Green's formulas make it possible to find also governing relations for internal moments (moments  $m_a^1$ ), and dislocation moments  $m_a^2$ :

$$m_i^1 = \frac{\partial U_V}{\partial \theta_i^1} = C^{11} \theta_i^1 + C^{12} \theta_i^2, \quad (27)$$

$$m_i^2 = \frac{\partial U_V}{\partial \theta_i^2} = C^{21} \theta_i^1 + k_v \theta_i^2.$$

The theorem is proved.

Further it will be shown that the governing relation for  $m_i^2$  gives the constitutive relation for the generalized heat flux. From the defining equation for temperature (25) we find

$$\theta^2 = \frac{T - K^{21} \theta^1}{K^{22}} = \frac{1}{K^{22}} T - \frac{K^{21}}{K^{22}} \theta^1. \quad (28)$$

Considering (28) we rewrite the equations of thermoelasticity and thermal conductivity in terms of displacements and temperature:

$$G_{ijmn} R_{m,nj} + (K^{11} - K^{12} \frac{K^{21}}{K^{22}}) R_{m,mi} - (C^{11} - C^{21} \frac{K^{21}}{K^{22}}) \Delta R_{m,mi} - \rho \ddot{R}_i + (\rho^{11} - \rho^{12} \frac{K^{21}}{K^{22}}) \ddot{R}_{m,mi} + \quad (29)$$

$$+ \frac{K^{12}}{K^{22}} T_{,i} - \frac{1}{K^{22}} C^{21} \Delta T_{,i} + \frac{\rho^{12}}{K^{22}} \ddot{T}_{,i} + P_i^V = 0,$$

$$(C^{21} K^{22} - C^{22} K^{21}) \Delta R_{k,k} + DK^{21} \dot{R}_{k,k} - (\rho^{21} K^{22} - \rho^{22} K^{21}) \ddot{R}_{k,k} - \quad (30)$$

$$- K^{22} T + C^{22} \Delta T - \rho^{22} \ddot{T} - D\dot{T} = 0.$$

We note that, as before, if in the equation (30) the term  $K^{22}T$  is considered small in the heat conduction operator  $-K^{22}T + C^{22}\Delta T - \rho^{22}\ddot{T} - D\dot{T}$ , then the heat equation (30) degenerates into the equation of hyperbolic heat conduction:

$$\begin{aligned} & C^{22} \Delta T - \rho^{22} \ddot{T} - D\dot{T} = \\ & = (C^{22} K^{21} - C^{21} K^{22}) \Delta R_{k,k} - (\rho^{22} K^{21} - \rho^{21} K^{22}) \ddot{R}_{k,k} - DK^{21} \dot{R}_{k,k}. \end{aligned} \quad (31)$$

In particular, for processes, in which there is no change of volume  $u_{k,k} = 0$ , the equation (31) takes the form of Maxwell-Cattaneo equation. Indeed, identifying the physical

constants in the equation (31) in accordance with the physical meaning, i.e. taking  $C^{22} = k_v$ ,  $\rho^{22} = \tau_v$ ,  $D = c_v$

we obtain the exact Maxwell-Cattaneo equation

$$k_v \Delta T - \tau_v \ddot{T} - c_v \dot{T} = 0,$$

here  $k_v$  is the thermal conductivity coefficient at a constant volume,  $\tau_v$  is the relaxation time of the heat flux at a constant volume,  $c_v$  is the specific heat capacity at a constant volume (the coefficient determining dissipation).

Consider the same heat conduction equation (30) and rewrite it in "stresses", i.e. in terms of temperature and pressure. Considering the governing relations (25), (26) we find:

$$R_{k,k} = \frac{1}{\left(K^{11} - \frac{K^{12}K^{21}}{K^{22}}\right)} p - \frac{\frac{K^{12}}{K^{22}}}{\left(K^{11} - \frac{K^{12}K^{21}}{K^{22}}\right)} T,$$

$$\theta^2 = \frac{\frac{K^{11}}{K^{22}}}{\left(K^{11} - \frac{K^{12}K^{21}}{K^{22}}\right)} T - \frac{\frac{K^{21}}{K^{22}}}{\left(K^{11} - \frac{K^{12}K^{21}}{K^{22}}\right)} p. \quad (32)$$

Taking into account the equalities (32), the heat equation (30) is written in the form:

$$\begin{aligned} & \left[ k_v + \frac{\frac{K^{12}}{K^{22}}(C^{22}K^{21} - C^{21}K^{22})}{\left(K^{11} - \frac{K^{12}K^{21}}{K^{22}}\right)} \right] \Delta T - \left[ \tau_v + \frac{\frac{K^{12}}{K^{22}}(\rho^{22}K^{21} - \rho^{21}K^{22})}{\left(K^{11} - \frac{K^{12}K^{21}}{K^{22}}\right)} \right] \ddot{T} - \left[ c_v + \frac{\frac{K^{12}}{K^{22}}DK^{21}}{\left(K^{11} - \frac{K^{12}K^{21}}{K^{22}}\right)} \right] \dot{T} = \\ & = \frac{1}{\left(K^{11} - \frac{K^{12}K^{21}}{K^{22}}\right)} (C^{22}K^{21} - C^{21}K^{22}) \Delta p - \frac{(\rho^{22}K^{21} - \rho^{21}K^{22})}{\left(K^{11} - \frac{K^{12}K^{21}}{K^{22}}\right)} \ddot{p} - \frac{DK^{21}}{\left(K^{11} - \frac{K^{12}K^{21}}{K^{22}}\right)} \dot{p}. \end{aligned}$$

From here you can immediately obtain the heat equation for isobaric processes and identify the corresponding physical constants:

$$k_p \Delta T - \tau_p \ddot{T} - c_p \dot{T} = 0, \quad (33)$$

where

$$k_p = k_v + \frac{\frac{K^{12}}{K^{22}}(C^{22}K^{21} - C^{21}K^{22})}{\left(K^{11} - \frac{K^{12}K^{21}}{K^{22}}\right)},$$

$$\tau_p = \tau_v + \frac{\frac{K^{12}}{K^{22}}(\rho^{22}K^{21} - \rho^{21}K^{22})}{\left(K^{11} - \frac{K^{12}K^{21}}{K^{22}}\right)}, \quad (34)$$

$$c_p = c_v + \frac{\frac{K^{12}}{K^{22}}DK^{21}}{\left(K^{11} - \frac{K^{12}K^{21}}{K^{22}}\right)}.$$

Taking into account the relations (34), as well as the equations of Hooke's law for pressure and temperature (25),(26) allows us to identify all the parameters of the generalized

model (20) and give a physical interpretation to the physical parameters of the general model, through known and measurable physical thermodynamic characteristics:

$$\begin{aligned}
K^{11} &= K_S, \quad K^{12} = -K_T \alpha c_V, \quad K^{21} = -\frac{K_S - K_T}{K_T \alpha}, \quad K^{22} = c_V, \\
K_T &= K^{11} - \frac{K^{12} K^{21}}{K^{22}}, \quad C^{21} = \frac{1}{\alpha c_V} k_p - \frac{K_S}{K_T} \frac{1}{\alpha c_V} k_V, \quad c_p = \frac{K_S}{K_T} c_V, \\
C^{11} &= C^{11}, \quad C^{12} = C^{21}, \quad C^{21} = \frac{1}{\alpha c_V} (k_p - \frac{K_S}{K_T} k_V), \quad C^{22} = k_V, \\
\rho^{21} &= \frac{1}{\alpha c_V} (\tau_p - \frac{K_S}{K_T} \tau_V), \quad \rho^{22} = \tau_V,
\end{aligned} \tag{35}$$

here  $K_S$ ,  $K_T$  are adiabatic and isothermal bulk moduli,  $k_V$ ,  $k_p$ ,  $c_V$ ,  $c_p$  are coefficients of thermal conductivity and heat capacity at constant volume and pressure, respectively,  $\tau_V$ ,  $\tau_p$  are relaxation times with constant volume and constant pressure,  $\alpha$  is thermal expansion coefficient.

Note that the presented interpretation of the model parameters is consistent with the known thermodynamic inequalities.

$$K_S - K_T > 0, \quad c_p - c_V > 0.$$

Finally, we consider the governing relations for dislocation moments  $m_a^2$  and rewrite it in terms of temperature and pressure using equalities (32). Defining the heat flux as

$$q_i = -c_V K_T m_i^2$$

we have

$$q_i = -k_p T_{,i} - (C^{21} c_V + \frac{K_S - K_T}{K_T \alpha} k_V) p_{,i}. \tag{36}$$

Note, that the generalized Hooke's law for the "temperature" double stress (heat flux) (36) takes the form of equation for the heat flux that was received in the in the recent work [33].

As a result, we showed that the methods of continuum mechanics allow us to obtain a variational model of an irreversible coupled thermodynamic process of dynamic thermoelasticity and hyperbolic thermal conductivity. At the same time, it is remarkable that the constitutive equations of the model are consistent with the known thermodynamic inequalities and include both the equations for the heat flux and the Duhamel-Neumann law.

## 5. Results and conclusion

Let's consider the model of gradient thermal conductivity (15), for which the use of variational methods of continuum mechanics was the basis for taking into account surface effects in the problem of thermomechanics. We assume that the parameters responsible for the effects of heat transfer at the boundary are equal to zero, i.e.  $a = b = 0$ . The parameter  $R_s$  is responsible for new, unexplored before surface effects that can not be described in the framework of the classical thermal conductivity, even taking into account surface effects such as surface tension, modifying the classical boundary conditions for heat flux (it can be shown that such is the parameter  $A^{11}$  in (11)). The parameter  $R_s$  appears only in the non-classical boundary condition for gradient theory.

Consider a one-dimensional stationary problem of heat conduction for two phases with the condition of a given constant heat flux at infinity. The solution of the heat conductivity equation of the gradient model (15) is represented as a superposition of two solutions –

"classical" solution  $\phi$  that satisfies the harmonic equation and the exponential solution of the Helmholtz equation  $\psi$ , characteristic of gradient theories

$$T = \phi - \psi, \quad \nabla^2 \phi = 0, \quad \nabla^2 \psi - l^{-2} \psi = 0, \quad (37)$$

where  $l$  is the scale parameter of the gradient model.

Contact conditions (see Eq.(15) that take into account the parameter  $R_s$  are written through the classical and exponential fields in the following form:

$$[T] = 0, \quad [\dot{T}] = 0, \quad [k \dot{\phi}] = 0, \quad [-k \psi] = R_s \dot{T}, \quad (38)$$

here  $k$  is the thermal conductivity coefficient; [...] denotes a jump of the function standing in them.

We argue that the parameter  $R_s$  allows one to model thermal resistance in heat transfer problems of inhomogeneous media. There is a statement.

**Theorem 3.**

1. The gradient model of thermal conductivity describes the effects of thermal resistance in the "classical" part of the temperature field, with a smooth continuous contact over the full temperature and its derivative at the contact boundary of the phases

2. The parameter of surface properties  $R_s < 0$ ... characterizes the thermal damage of the surface and the effect of a jump in the total temperature in the vicinity of the contact boundary of the phases, i.e. thermal resistance of the boundary and the Kapitza effect distributed over the interfacial zone

**Proof.** In the one-dimensional case, we obtain the following simple representations for the solution with unknown coefficients, which we will find from the contact conditions:

$$\phi = A_i + B_i x, \quad \psi = A_i^* e^{-x/l_i} + B_i^* e^{x/l_i}, \quad (i = 1, 2). \quad (39)$$

Then, taking into account Eqs (37), (39) and the decreasing of the gradient part of solution at infinity we have the following solution for a two-phase medium:

$$T = A_1 + B_1 x - A_1^* e^{x/l_1}, \quad x < 0, \quad T = A_2 + B_2 x - A_2^* e^{-x/l_2}, \quad x > 0. \quad (40)$$

Unknown coefficients in solutions (40) are found from the conditions of contact of the phases (38):

$$B_1 = -\frac{q}{\kappa_1}, \quad B_2 = -\frac{q}{\kappa_2}, \quad A_1^* = -q \frac{l_1 R_s + l_2 (\kappa_2 - \kappa_1)}{\kappa_1 R_s + l_1 \kappa_1 + l_2 \kappa_2}, \quad A_2^* = -q \left( \frac{l_2}{\kappa_1} \frac{(l_1 + l_2) \kappa_1}{R_s + l_1 \kappa_1 + l_2 \kappa_2} - \frac{l_2}{\kappa_2} \right),$$

where  $q$  is the value of a given heat flux,  $l_i$ ,  $i = 1, 2$ , are the scale gradient parameters of a two-layer medium.

As a result, we find a jump in the classical component of the temperature at the phase boundary, while the total temperature and its derivative are continuous at the contact boundary.

$$[\phi] = A_2 - A_1 = A_2^* - A_1^* = q \frac{R_s (l_1/\kappa_1 + l_2/\kappa_2) + l_1 l_2 (\kappa_1/\kappa_2 + \kappa_2/\kappa_1 - 2)}{R_s + l_1 \kappa_1 + l_2 \kappa_2}. \quad (41)$$

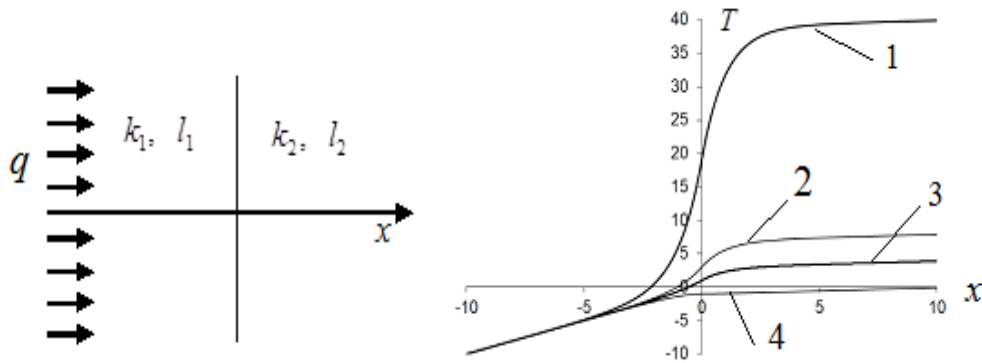
In particular, when  $l_1 = l_2 = l$  we get

$$[\theta] = \frac{lq (1 + \kappa_1/\kappa_2) R_s / \kappa_2 + l(1 - \kappa_1/\kappa_2)^2}{\kappa_1 R_s / \kappa_2 + l(1 + \kappa_1/\kappa_2)}.$$

The resulting relation (41) proves the theorem. Indeed, solution (41) shows that a jump in the harmonic part of the temperature at the phase boundary occurs at  $R_s < 0$ , depends on the quantity  $R_s$ . and is proportional to the heat flux, as the Kapitza effect shows [29].

The theorem is proved.

Consequently, the gradient model of thermal conductivity allows us to simulate thermal resistance for the "classical" part of the temperature. Note, that at the phase boundary, the continuity of the total temperature and its derivative takes place. When  $R_s > 0$ , the jump is proportional to the small scale parameter, and the gradient model of thermal conductivity as a whole allows one to simulate the effects of an anomalous increase in the effective thermal conductivity for multiphase materials if the inclusions have a high thermal conductivity even in the case of low thermal conductivity of the matrix. These effects are due to the properties of the interfacial layers in the vicinity of the contact boundaries of the phases, which is characteristic for gradient theories. It is easy to verify that in the case of  $R_s < 0$ , the parameter  $R_s$  can describe the phase boundaries with an arbitrary given jump in the classical part of the temperature field up to a singularity, which indicates that the boundary is so damaged that heat transfer is impossible. Figure 1 shows the temperature distribution lines for  $k_2 = 10 \left[ \frac{W}{m \cdot K} \right]$ ,  $k_1 = 1 \left[ \frac{W}{m \cdot K} \right]$ ,  $q = -1 \left[ \frac{W}{m^2} \right]$ ,  $l_1 = l_2 = l$  and different values of  $R_s$ :



**Fig 1.** Effects of thermal resistance in the vicinity of the contact boundary of the phases  
 1 –  $R_s/lk_2 = -1.09$  (significant contact boundary resistance),  
 2 –  $R_s/lk_2 = -1.05$ , 3 –  $R_s/lk_2 = -1$ , 4 –  $R_s/lk_2 = 10$

As a second example, consider the problem of determining the effective thermal conductivity  $\tilde{k}$  of a composite with spherical inclusions, taking into account gradient effects and effects of thermal resistance, if the thermal conductivity coefficient of the matrix is equal to  $k_1$  and the thermal conductivity coefficient of the inclusion is equal to  $k_0$ . In this case, the solution is constructed as a superposition of a uniform field and radial factors with unknown coefficients [34]:

$$\phi = (A_i + r^{-3}B_i)z, \quad \psi = (h_1(r)A_i^* + \hat{h}_1(r)B_i^*)z,$$

$$h_1(r) = \frac{1}{r} \frac{d}{dr} \left( \frac{\sinh(r/l)}{r} \right) = \frac{\cosh(r/l)(r/l) - \sinh(r/l)}{r^3},$$

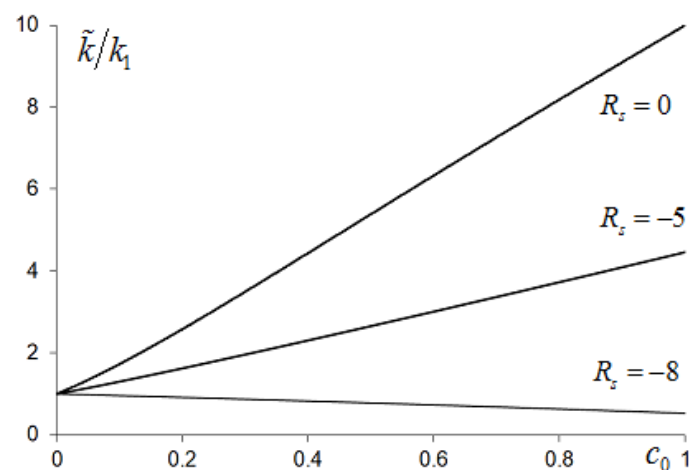
$$\hat{h}_1(r) = \frac{1}{r} \frac{d}{dr} \left( \frac{\cosh(r/l)}{r} \right) = \frac{\sinh(r/l)(r/l) - \cosh(r/l)}{r^3}.$$

For the spherical inclusion of the radius  $r_0$  and the spherical layer (matrix) of the radius  $r_1$ , we have the following representation for the temperature, taking into account the decrease of the exponential field at infinity:

$$T = (A_0 - h_1^{(0)}(r)A_0^*)z, \quad r < r_0,$$

$$T = \left( A_1 + r^{-3} B_1 - h_1^{(1)}(r) A_1^* - \hat{h}_1^{(1)}(r) B_1^* \right) z, \quad r_0 < r < r_1, \quad T = (1 + r^{-3} B_2) z, \quad r_1 < r.$$

The algorithm for determining the effective thermal conductivity takes into account considerations of equivalent homogeneity in the model of three spherical bodies. From here we obtain the condition  $B_2 = 0$  in an efficient media. Contact conditions at the border allow you to find all the coefficients taking into account the thermal resistance  $R_s$ . Figure 2 shows the dependence of the effective thermal conductivity  $\tilde{k}$  on the concentration of inclusions.  $c_0 = (r_0/r_1)^3$  when  $k_0/k_1 = 10$ ,  $l_0/r_0 = l_1/r_1 = 1$  and different thermal resistance coefficients  $R_s/lk_1$ .



**Fig. 2.** Effective thermal conductivity of a composite with spherical inclusions. Accounting for thermal resistance in the model of the gradient stationary thermal conductivity

We see that the gradient thermal conductivity ( $R_s = 0$ ) allows one to simulate the effects of a significant increase in the effective thermal conductivity even in the case of small volume contents of inclusions. Estimates show that the effect of "amplification" essentially depends on the size of the inclusions, i.e. there is a scale effect in thermal conductivity. On the other hand, negative values of the parameter  $R_s$  that we introduced here as surface properties parameter make it possible to simulate a significant decrease in the effective thermal conductivity, which is explained by the influence of the temperature damage of the contact boundary of the phases.

In conclusion, we note that this paper demonstrated the possibility of using the methods of continuum mechanics to simulate coupled thermodynamic processes, including the stationary and dynamical, reversible and irreversible processes. Variational approaches of mechanics lead to the possibility of expanding models of thermoelasticity and thermal conductivity by taking into account connectivity, attracting non-local models, models of dissipation channels and models of surface interactions.

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