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Uncertainties in the heat conduction problems and reliable estimates*

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Abstract

The heat conduction problems for anisotropic bodies are studied taking into account the uncertainties in the material orientation. The best estimations of the upper and lower bounds of the considered energy dissipation functional are based on the developing new approach consisting in solution of some optimization problems and finding the extremal internal material structures, which realize minimal and maximal dissipation.

1 Introduction

The problems of incompleteness of data and uncertainties are typical for anisotropic solids and structures having chaotic orientation of small material particles such as grains, crystal or short nano-fibers. Different possible compositions of elementary particles with various orientations result in different values of such integral characteristics as a total dissipation energy in the heat conduction problems, total potential energy in the thermoelasticity and thermoconductivity problems. Taking into account the conditions of uncertainties concerning the material orientations it is very important to obtain various estimations of the considered functionals and in particular limiting estimates known as double-side or bilateral estimates Banichuk and Neittaanmäki (2010).

In the proposed article the problem of estimation of dissipation energy characteristics is considered for anisotropic body constituting of the locally orthotropic material. It is assumed that an orientation of the principle axes of orthotropy is not known beforehand at each point of the body and can be distributed by various ways in different parts of the body including chaotic orientation. The search for double-side estimates is reduced to the solution of optimization problems and finding the extremal orientations of the orthotropy axes.

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2 Heat conduction problem for bodies from locally orthotropic material

Let us consider heat conduction problem for solid body occupied the domain Ω (see Figure 1) with the boundary $\Gamma = \Gamma_g + \Gamma_i$ ($\Gamma_g \cap \Gamma_i = 0$). The material of the body is anisotropic with respect to the heat conduction process described by the known relations Landau and Lifshitz (1965), Berdichevsky (2009), Nowacki (1970)

$$\mathbf{q} = D \cdot \nabla \varphi, \quad \varphi = \theta^{-1} \quad (1)$$

where θ is a temperature, \mathbf{q} is a vector of the heat flux and D is a heat conduction tensor of the second rank. In the case of absence of the source of heat in the domain Ω we will use the boundary conditions, governing equation and the quality functional (dissipation of energy) in the following form

$$(\varphi)_{\Gamma_g} = \varphi^0, \quad (\mathbf{n} \cdot D \cdot \nabla \varphi)_{\Gamma_i} = 0 \quad (2)$$

$$\nabla \cdot (D \cdot \nabla \varphi) = 0 \quad x \in \Omega \quad (3)$$

$$J = \int_{\Omega} \nabla \varphi \cdot D \cdot \nabla \varphi d\Omega \quad (4)$$

where φ^0 is a given function specified on Γ_g , \mathbf{n} is an outwards unit normal vector specified on the part Γ_i , (\cdot) between the vectors means the scalar product and the symbol ∇ is the gradient operator, i.e.

$$\nabla \varphi = \left\{ \frac{\partial \varphi}{\partial x_1}, \frac{\partial \varphi}{\partial x_2}, \frac{\partial \varphi}{\partial x_3} \right\}.$$

In accordance with the variational principle Berdichevsky (2009) the actual distribution of the function φ realizes a minimum for the functional J on the set of admissible functions satisfying the first boundary condition in (2), if

$$J \rightarrow \min_{\varphi} \quad (5)$$

Note the second boundary condition in the (2) plays the role of transversality condition for the functional (4) and is satisfied "automatically" for extremum solution. Note that the equation (3) is the Eulerian equation for the functional (4).

In what follows we will suppose that the material is locally orthotropic and the orientation of the axes of orthotropy is unknown beforehand. Let us fix the unit vectors $\mathbf{e}_1^0, \mathbf{e}_2^0, \mathbf{e}_3^0$ of orthogonal coordinate system x_1, x_2, x_3 which is considered as a global system (see Figure 2). The principal directions unit vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ of the heat conduction tensor D of orthotropic material (axes of local symmetry) at the arbitrary point $(x_1, x_2, x_3) \in \Omega$ are related with the global coordinate vectors $\mathbf{e}_1^0, \mathbf{e}_2^0, \mathbf{e}_3^0$ by means of the rotation tensor $Q = Q(x)$ as

$$\mathbf{e}_i = Q * \mathbf{e}_i^0 = Q \cdot \mathbf{e}_i^0 \quad (i = 1, 2, 3) \quad (6)$$

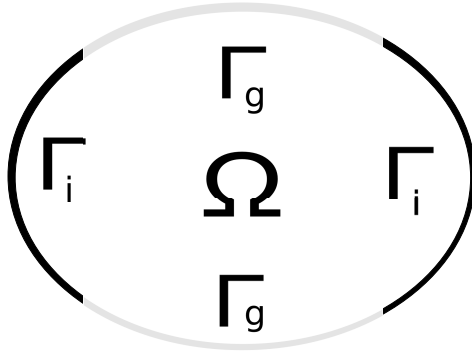


Figure 1: Domain Ω with given temperature Γ_i (black) and thermally insulated Γ_g (grey) boundary conditions.

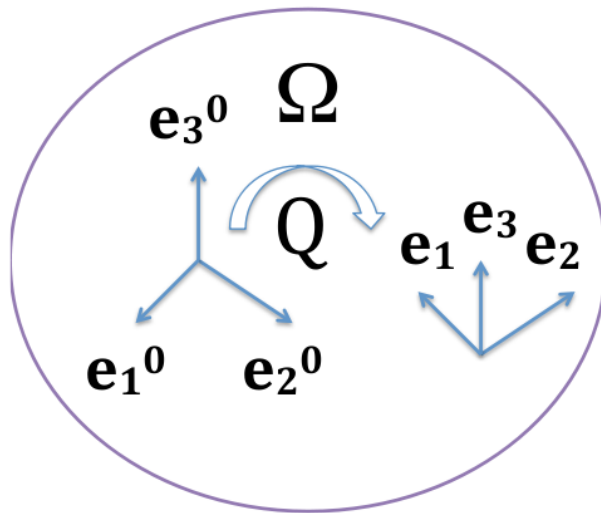


Figure 2: Transformation of global unit vectors to the local material principle vectors by rotation tensor Q .

$$Q^T \cdot Q = Q \cdot Q^T = E \quad (7)$$

where the symbol T means the operation of transposition and $E = \{\delta_{ij}\}$ - unit tensor, where δ_{ij} is a Kronecker symbol ($i, j = 1, 2, 3$) and $(*)$ is a tensor operation of the rotation. In the axes of symmetry of the orthotropic material the heat conduction tensor D is written as

$$D = D_{ij} \mathbf{e}_i \otimes \mathbf{e}_j = D_{ij}^0 Q \cdot \mathbf{e}_i^0 \otimes Q \cdot \mathbf{e}_j^0 = Q * (D_{ij}^0 \mathbf{e}_i^0 \otimes \mathbf{e}_j^0) = Q * D^0 \quad (8)$$

where \otimes is tensor product and

$$D^0 = D_{ij}^0 \cdot \mathbf{e}_i^0 \otimes \mathbf{e}_j^0 \quad (9)$$

The expression for the heat conduction tensor D can be rewritten in the form

$$D = D_{ij}^0 Q \cdot \mathbf{e}_i^0 \otimes Q \cdot \mathbf{e}_j^0 = Q \cdot (D_{ij}^0 \mathbf{e}_i^0 \otimes \mathbf{e}_j^0) \cdot Q^T = Q \cdot D^0 \cdot Q^T \quad (10)$$

If \varkappa_i and \mathbf{e}_i^0 i.e. eigenvalues and eigenvectors of the tensor D^0 , i.e.

$$D^0 \cdot \mathbf{e}_i^0 = \varkappa_i^0 \mathbf{e}_i^0 \quad (11)$$

then \varkappa_i and $\mathbf{e}_i = Q \cdot \mathbf{e}_i^0$ i.e. eigenvalues and eigenvectors of the tensor $D = Q * D^0$, i.e.

$$D \cdot \mathbf{e}_i = \varkappa_i \mathbf{e}_i \quad (12)$$

Taking into account the equations (7), (8) and (11) we will have the equation (12). In fact

$$D \cdot \mathbf{e}_i = (Q * D^0) \cdot (Q \cdot \mathbf{e}_i^0) = Q * (D^0 \cdot \mathbf{e}_i^0) = \varkappa_i^0 Q \cdot \mathbf{e}_i^0 = \varkappa_i \mathbf{e}_i \quad (13)$$

For given tensor D^0 the values of the functionals J depend on the realization of $Q = Q(x)$ and corresponding actual values of $\varphi = \varphi(x)$, minimizing the functional of energy dissipation (4) under constraints (2) (for considered $Q(x)$, i.e.

$$J(Q, \varphi_*) = \min_{\varphi} J(Q, \varphi) \quad (14)$$

3 Uncertainties in orientation of orthotropic material and double-side estimates

If there is no data concerning material orientation, i.e. the tensor-function $Q = Q(x)$ ($x \in \Omega$), characterizing materia distribution is unknown, then it is very important to obtain the lower and upper bounds of J , i.e. to find the limit double-side estimates J_{\min} and J_{\max} , such that

$$J_{\min} \leq J(Q, \varphi_*) \leq J_{\max} \quad (15)$$

for any realization of Q satisfying the condition (7).

To obtain reliable estimations of the dissipation energy functional J and other important characteristics we apply in the paper an approach based on the solution

of two optimization problems. The following problem is devoted to finding the lower estimate

$$J_{\min} = \min_Q J(Q, \varphi_*) = \min_Q \min_{\varphi} J(Q, \varphi) \quad (16)$$

and another problem consists in the searching of the upper bounds

$$J_{\max} = \max_Q J(Q, \varphi_*) = \max_Q \min_{\varphi} J(Q, \varphi) \quad (17)$$

where min and max with respect to Q in the equations (16) and (17) are determined under constraint (7). Operation min with respect to φ in the equations (16) and (17) is performed taking into account boundary conditions from the equation (2).

In what follows we will study the proposed approach and problems of searching the extremum of J with respect to Q

$$J \rightarrow \text{extr}_Q \quad (18)$$

and analyze extremum conditions and behavior equations.

4 Extremal conditions for orthotropic material orientation

To derive extremum conditions defining the orthogonal tensor of rotation $Q = Q(x)$ and characterizing the extremal orientations of orthotropy axes let us use the method of Lagrange multipliers and construct augmented functional

$$J^L = J + J_P \quad (19)$$

$$J_P = \int_{\Omega} P \cdot \cdot (Q^T \cdot Q - E) \, d\Omega \quad (20)$$

$$J = \int_{\Omega} \nabla\varphi \cdot (Q * Q^0) \cdot \nabla\varphi \, d\Omega = \int_{\Omega} \nabla\varphi \cdot (Q \cdot D^0 \cdot Q^T) \cdot \nabla\varphi \, d\Omega \quad (21)$$

where $(\cdot\cdot)$ between tensors mean double scalar product and symmetric tensor of second rank $P = P(x)$ ($x \in \Omega$) is Lagrange multiplier, specifying in Ω and corresponding to the condition of orthogonality (see equation (7)). The dissipation energy functional J can be also rewritten as

$$J = \int_{\Omega} B \cdot \cdot (Q \cdot D^0 \cdot Q^T) \, d\Omega \quad (22)$$

Here by means of B we denote the following symmetric second rank tensor

$$B = \nabla\varphi \otimes \nabla\varphi, \quad B^T = B \quad (23)$$

and the symbol \otimes is the tensor product.

Let us derive the following expressions for the first variations δJ and δJ_P with respect to variation δQ of rotation tensor Q . We will have

$$\delta J = \int_{\Omega} B \cdot \cdot (\delta Q \cdot D^0 \cdot Q^T + Q \cdot D^0 \cdot \delta Q^T) \, d\Omega = 2 \int_{\Omega} \delta Q \cdot \cdot (D^0 \cdot Q^T \cdot B) \, d\Omega \quad (24)$$

and

$$\delta J_P = \int_{\Omega} P \cdot \cdot (\delta Q^T \cdot Q + Q^T \cdot \delta Q) \, d\Omega = 2 \int_{\Omega} \delta Q \cdot \cdot (P \cdot Q^T) \, d\Omega \quad (25)$$

Taking into account the expressions (19) – (21), (24) and (25) we will find the expression for the total variation δQ in the following form

$$\delta J^L = \delta J + \delta J_P = 2 \int_{\Omega} \delta Q \cdot \cdot (D^0 \cdot Q^T \cdot B + P \cdot Q^T) \, d\Omega \quad (26)$$

Using the extremum condition

$$\delta J^L = 0 \quad (27)$$

and arbitrariness of Q , i.e. arbitrariness of δQ , we will have

$$D^0 \cdot Q^T \cdot B + P \cdot Q^T = 0, \quad x \in \Omega \quad (28)$$

Multiplying the relation (28) on Q and using formulae (10) and (23) we find

$$D \cdot \nabla \varphi \otimes \nabla \varphi = -Q \cdot P \cdot Q^T, \quad x \in \Omega \quad (29)$$

This relation means the symmetry of the second rank tensor

$$(D \cdot \nabla \varphi) \otimes \nabla \varphi$$

written in the left hand side of the equality (29), i.e.

$$(D \cdot \nabla \varphi) \otimes \nabla \varphi = \nabla \varphi \otimes (D \cdot \nabla \varphi) \quad (30)$$

The equality (30) is satisfied if the vectors $D \cdot \nabla \varphi$ and $\nabla \varphi$ are parallel, i.e.

$$D \cdot \nabla \varphi = \lambda \nabla \varphi \quad (31)$$

where λ is some scalar value.

5 Double-side estimates based on derived extremal conditions

The necessary extremum condition (31) for dissipation energy functional J with respect to rotation tensor Q , defining an extremal distribution of Q and expressing the collinearity of the vectors $\nabla \varphi$ and

$$D \cdot \nabla \varphi = (Q \cdot D \cdot Q^T) \cdot \nabla \varphi$$

is an eigenvalue problem. Consequently, the vector $\nabla\varphi$ is one of the eigenvectors of the heat conduction tensor D :

$$D \cdot \nabla\varphi = \lambda_i \nabla\varphi, \quad i = 1, 2, 3 \quad (32)$$

Taking into account that the eigenvalues λ_i of the tensors D and D^0 are equal (see the equations (11) and (13)) and given, we assume

$$\lambda_1 = \lambda_{\min} < \lambda_2 < \lambda_3 = \lambda_{\max} \quad (33)$$

Substituting (32) into the Euler equation (3) of the functional J we obtain the equations that determine the stationary distribution of scalar function $\varphi = \varphi(x)$:

$$\nabla \cdot (\lambda_i \nabla\varphi) = 0, \quad (i = 1, 2, 3), \quad x \in \Omega \quad (34)$$

in the case of specified rotation tensor Q according to the equation

$$(Q \cdot D^0 \cdot Q^T) \cdot \nabla\varphi = \lambda_i \nabla\varphi \quad (35)$$

The elliptical partial differential equation (34) with the boundary conditions

$$(\varphi)_{\Gamma_g} = \varphi^0, \quad (\lambda_i \mathbf{n} \cdot \nabla\varphi)_{\Gamma_i} = 0 \quad (36)$$

corresponding to conditions (2) with the relations (32) constitute the conventional boundary value problem describing, as it is well known, homogeneous or nonhomogeneous isotropic processes of the heat conductivity. Under some known additional constraints superimposed on the boundary shape $\Gamma = \Gamma_g + \Gamma_i$ ($\Gamma_g \cap \Gamma_i = 0$) we have the existence and uniqueness of the solution of (34) and (36) with given λ_i .

If we assume that the same way of extremum orientation of the principle axes of orthotropy is realized for all domain Ω , then λ_i is constant in Ω and the considered heat conduction process is described by the classical boundary value problem

$$\Delta\varphi = 0, \quad x \in \Omega \quad (37)$$

$$(\varphi)_{\Gamma_g} = \varphi^0, \quad (\mathbf{n} \cdot \nabla\varphi)_{\Gamma_i} = 0 \quad (38)$$

for Laplace equation with mixed (in general case) boundary conditions. Here Δ is a Laplace operator acting in 3-dimensional space.

Note that the equality in the equation (37) means that in the case of the body with extremum orthotropy the heat conduction process is described by the same equation as in the isotropic case. If the domain Ω consists of several sub-domains Ω_i such that

$$\Omega = \cup \Omega_i, \quad \Omega_i \cap \Omega_j = 0 \quad (i \neq j) \quad (39)$$

and for each separate sub-domain Ω_i the same extremum way of material orientation is taken, then the isotropic heat conduction process is realized for all considered subdomains.

Let us assume that the orthotropic material is distributed in accordance with the same extremum rule in the domain Ω . Then we will have the "isotropic" boundary

value problem (37) and (38), and consequently the state variable φ (inverse temperature) is independent of λ_i . As a result we obtain the following minimal and maximal values of the considered quality functional J :

$$\min_Q J = \lambda_{\min} I \quad (40)$$

$$\max_Q J = \lambda_{\max} I \quad (41)$$

where

$$I = \int_{\Omega} (\nabla\varphi)^2 d\Omega \quad (42)$$

Thus the double-side estimates of the energy dissipation functionals can be written as

$$\lambda_{\min} \leq \frac{J}{I} \leq \lambda_{\max} \quad (43)$$

6 Two-dimensional case of extremal material orientation

Separately consider the two-dimensional case with plane domain Ω . In this case

$$\nabla\varphi = \left\{ \frac{\partial\varphi}{\partial x_1}, \frac{\partial\varphi}{\partial x_2} \right\}, \quad x = \{x_1, x_2\} \in \Omega \quad (44)$$

Then the element of orthogonal tensor Q are represented in the form

$$Q_{11} = Q_{22} = \cos \alpha \quad Q_{21} = -Q_{12} = \sin \alpha \quad (45)$$

where α is the angle of rotation of the specified tensor Q . On the basis of the equation (35) we obtain an explicit expression relating the angle $\alpha = \alpha(x_1, x_2)$ with the function $\varphi = \varphi(x_1, x_2)$. For definiteness assume that the vector $\nabla\varphi$, presented in the equation (44), correspond to the eigenvalue λ_i . Then the eigenvector \mathbf{k} , corresponding to the eigenvalue $\lambda_j (i \neq j)$ is

$$\mathbf{k} = \left\{ \frac{\partial\varphi}{\partial x_2}, -\frac{\partial\varphi}{\partial x_1} \right\} \quad (46)$$

which is orthogonal to the eigenvector $\nabla\varphi$ from the equation (44). We form a scalar product of both sides of the vector equality (32) with the vector \mathbf{k} . We will have

$$\mathbf{k} \cdot D \cdot \nabla\varphi = 0 \quad (47)$$

This relation contains two separate cases. The first case:

$$\cos 2\alpha = C, \quad \sin 2\alpha = S \quad (48)$$

where

$$C = -\frac{(D_{11}^0 - D_{22}^0) \left\{ \left(\frac{\partial \varphi}{\partial x_1} \right)^2 - \left(\frac{\partial \varphi}{\partial x_2} \right)^2 \right\} + 4D_{12}^0 \frac{\partial \varphi}{\partial x_1} \frac{\partial \varphi}{\partial x_2}}{(\nabla \varphi)^2 \sqrt{(D_{11}^0 - D_{22}^0)^2 + 4(D_{12}^0)^2}} \quad (49)$$

and

$$S = \frac{2(D_{11}^0 - D_{22}^0) \frac{\partial \varphi}{\partial x_1} \frac{\partial \varphi}{\partial x_2} - 2D_{12}^0 \left\{ \left(\frac{\partial \varphi}{\partial x_1} \right)^2 - \left(\frac{\partial \varphi}{\partial x_2} \right)^2 \right\}}{(\nabla \varphi)^2 \sqrt{(D_{11}^0 - D_{22}^0)^2 + 4(D_{12}^0)^2}} \quad (50)$$

corresponds to the smaller eigenvalue $\lambda_1 (\lambda_1 < \lambda_2)$. The second case:

$$\cos 2\alpha = -C, \quad \sin 2\alpha = -S \quad (51)$$

corresponds to the larger eigenvalue $\lambda_2 (\lambda_2 > \lambda_1)$.

7 Examples of double-side estimates

Suppose at first that the orthotropic material occupies the 3-dimensional domain Ω situated between the internal sphere of radius r_1 , where $r_1, r_2 (r_1 < r_2)$ is given values. The temperature of $\theta = \theta_1$ is defined at the internal boundary and the temperature $\theta = \theta_2$ is given at the external boundary, where $\theta_1 < \theta_2$. Note that $\theta_i, (i = 1, 2)$ are given and positive values. Thus we consider the following boundary conditions

$$\begin{aligned} \varphi = \varphi_1 = \frac{1}{\theta_1}, \quad r = r_1 \\ \varphi = \varphi_2 = \frac{1}{\theta_2}, \quad r = r_2 \end{aligned} \quad (52)$$

where $\varphi_1 < \varphi_2$. Here we use spherical coordinate system with the origin at $r = 0$. From the properties of symmetry it follows that the extremum orientations of the axes of orthotropy with

$$\lambda_1 = \lambda_{\min} \quad \text{and} \quad \lambda_3 = \lambda_{\max}$$

corresponding respectively to the cases

$$J \rightarrow \min_Q \quad \text{and} \quad J \rightarrow \max_Q$$

are realized in radial direction. Besides, the gradient of φ , i.e. vector $\nabla \varphi$, and also the heat flux vector \mathbf{q} are directed along the radius vector at each point of the domain Ω . Note that the heat flux \mathbf{q} is absent in circumferential directions. The following values characterize the extremal distribution of material:

$$\mathbf{q}_{\min} = \lambda_{\min} N \mathbf{r}_0, \quad \mathbf{q}_{\max} = \lambda_{\max} N \mathbf{r}_0 \quad (53)$$

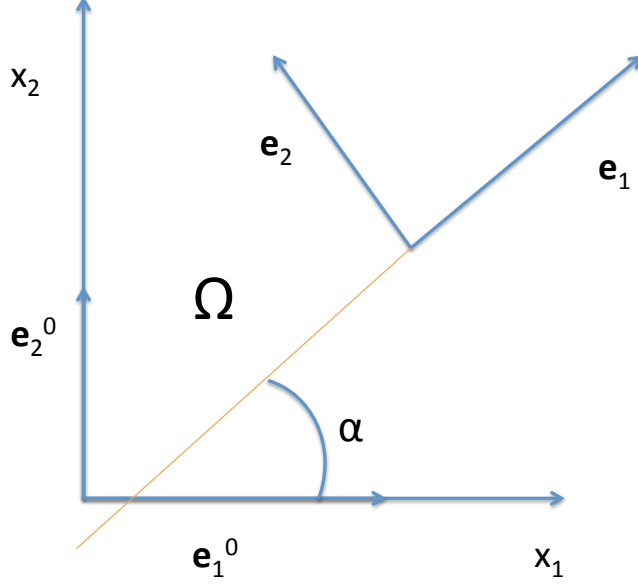


Figure 3: Orientation of local orthotropy in 2-dimensional case.

$$\lambda_{\min} I \leq J \leq \lambda_{\max} I$$

$$N = \frac{\varphi_2 - \varphi_1}{r_2 - r_1}, \quad \mathbf{r}_0 = \frac{\mathbf{r}}{|\mathbf{r}|}$$

where

$$I = \int_{\Omega} (\nabla \varphi)^2 d\Omega = \frac{4}{3} \pi N (\varphi_2 - \varphi_1) (r_1^2 + r_1 r_2 + r_2^2) \quad (54)$$

and \mathbf{r}_0 is an unit vector, oriented in radial direction.

Next let us consider the problem of finding the double-side estimates when a simply connected domain Ω occupied by the orthotropic material is a rectangular parallelepiped with the upper and lower faces at $x_3 = -c$ and $x_3 = c$ and side faces at $x_1 = \pm a$ and $x_2 = \pm b$. We use Cartesian coordinate system (x_1, x_2, x_3) and we assume that the temperature θ is given at the lower and upper faces and the sidefaces are thermally insulated, i.e. the boundary conditions have the form:

$$\varphi = \varphi_1 = \frac{1}{\theta_1}, \quad x_3 = -c \quad \text{and} \quad \varphi = \varphi_2 = \frac{1}{\theta_2}, \quad x_3 = c \quad (55)$$

and

$$\mathbf{q} \cdot \mathbf{n} = \mathbf{n} \cdot \mathbf{D} \cdot \nabla \varphi = 0 \text{ at } x_1 = \pm a, x_2 = \pm b \quad (56)$$

where $\theta_1 > 0$, $\theta_2 > 0$ and $(\theta_1 > \theta_2)$. Extremal material distribution and corresponding heat conduction processes are characterized by the existence of level surfaces x_3 is constant ($-c < x_3 < c \in \Omega$) with a constant distribution of variable φ (constant temperature θ). The gradient of φ is parallel to x -axis. Therefore the axes of orthotropy with minimal eigenvalue $\lambda = \lambda_{\min}$ (in the case $J \rightarrow \min_Q$) and with maximal eigenvalue $\lambda = \lambda_{\max}$ (in the case of $J \rightarrow \max_Q$) are oriented in a parallel way with respect to the axis x_3 . Such orientation provides, respectively, either the minimum or the maximum of dissipation. For considered problem we will have

$$\begin{aligned} \mathbf{q}_{\min} &= \lambda_{\min} \Phi \mathbf{x}_3^0, & \mathbf{q} &= \lambda_{\max} \Phi \mathbf{x}_3^0 & (57) \\ \min_Q J &= \lambda_{\min} I, & \max_Q J &= \lambda_{\max} I \\ \Phi &= \frac{\varphi_2 - \varphi_1}{2c}, & \nabla \varphi &= \Phi \mathbf{x}_3^0, & \mathbf{x}_3^0 &= \frac{\mathbf{x}_3}{|\mathbf{x}_3|} \end{aligned}$$

where

$$I = \int_{\Omega} (\nabla \varphi)^2 d\Omega = \frac{2ab}{c} (\varphi_2 - \varphi_1)^2 \quad (58)$$

and \mathbf{x}_3^0 is a unit vector of the x_3 -axis, obtained when the vector \mathbf{x}_3 is divided by its length $|\mathbf{x}_3|$.

8 Notes and conclusion

In the case, when the coefficient D_{ij} and the considered eigenvalues λ_i are independent of $x = (x_1, x_2, x_3)$, then the anisotropic behaviour equation is reduced to the Laplace equation which describes the heat conduction of homogeneous isotropic body. Since the theory of the heat conduction of isotropic homogeneous solids is well developed and solution of the corresponding boundary value problem has been found (analytically and numerically) for most problems of practical importance, then this reduction allows to consider the above problem of obtaining of double-side estimates to be solved.

Taking into account the conditions of uncertainties concerning material orientations we obtain various estimations of the considered functionals and in particular limiting estimates known as double-side or bilateral estimates. The search of double-side estimates as it was shown is reduced to the solution of optimization problems and finding the extremal orientation of the orthotropy axes.

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