Numerical Simulation of Thermoelasticity Problems on High Performance Computing Systems

Petr V. Sivtsev[1(✉)], Petr N. Vabishchevich[2], and Maria V. Vasilyeva[1]

[1] North-Eastern Federal University, 58, Belinskogo, 677000 Yakutsk, Russia
sivkapetr@mail.ru

[2] Nuclear Safety Institute, 52, B. Tulskaya, 115191 Moscow, Russia

Abstract. In this work we consider the coupled linear system of equations for temperature and displacements which describes the thermoelastic behaviour of the body. For numerical solution we approximate our system using finite element method. As model problem for simulation we consider the thermomechanical state of the ceramic substrates with metallization, which are used for the manufacturing of light-emitting diode modules. The results of numerical simulation of the 3D problem in the complex geometric area are presented.

1 Introduction

Many applied problems of mathematical modeling are connected with the calculation of the stress-strain state of solids. In many cases, the deformation is caused by thermal expansion. The thermoelasticity models are used for their research.

Basic mathematical models include heat conduction equation and Lame thermoelasticity equation for displacements [1–4]. The fundamental point is that the system is tied up, the equation for displacement comprises volumetric force proportional to the temperature gradient and the temperature equation includes a term that describes the compressibility of the medium.

In this work we consider the coupled linear system of equations for temperature and displacements which describes the thermoelastic behavior of the body. For numerical solution we approximate our system using finite element method [5–10].

As model problem we consider simulation of the thermomechanical state of the ceramic substrates with metallization, which are used for the manufacturing of light-emitting diode (LED) modules. The results of numerical simulation of the 3D problem in the complex geometric area are presented. Calculations are performed using the North-Eastern Federal University computational cluster *Arian Kuzmin*.

2 Problem Statement

Under mechanical and thermal effects in an elastic body displacement $\boldsymbol{u}$, strain $\boldsymbol{\varepsilon}$ and stress $\boldsymbol{\sigma}$ occur in an elastic body. Let T be the constant absolute temperature

I. Dimov et al. (Eds.): FDM 2014, LNCS 9045, pp. 364–370, 2015.
DOI: 10.1007/978-3-319-20239-6_40

at which body is in initial state of equilibrium, and θ be temperature increment. External forces that impact the body are treated as mechanical effects, whereas for the thermal influences one realizes heat exchange processes between the body surface and environment, and release or absorption of heat by the sources inside the body.

Mathematical model of thermoelastic state is defined by coupled system of equations for displacement $\boldsymbol{u}$ and temperature increment θ in domain Ω [1–4]:

$$-\mathrm{div}\,(k\,\mathrm{grad}\,\theta) = f. \tag{1}$$

$$-\mu\Delta\boldsymbol{u} - (\lambda+\mu)\,\mathrm{grad}\,\mathrm{div}\boldsymbol{u} + \alpha\,\mathrm{grad}\,\theta = 0, \tag{2}$$

Here μ, λ are Lame constants, k is heat conduction coefficient, c is strain-free volumetric heat capacity, $\alpha = \alpha_T(3\lambda+2\mu)$, where α_T is linear thermal expansion coefficient, $\boldsymbol{\varepsilon}$ is strain tensor:

$$\boldsymbol{\varepsilon} = \frac{1}{2}(\boldsymbol{\nabla u} + (\boldsymbol{\nabla u})^T),$$

and $\boldsymbol{\sigma}$ is stress tensor:

$$\boldsymbol{\sigma} = \lambda\boldsymbol{\nabla u I} + 2\mu\boldsymbol{\varepsilon}.$$

Here $\boldsymbol{I}$ defines unit tensor.

Also Eqs. (1) and (2) are supplemented with appropriate boundary conditions:

$$\begin{aligned} \boldsymbol{\sigma n} &= 0, \quad \boldsymbol{x} \in \Gamma_N^u, \quad \boldsymbol{u} = \boldsymbol{u}_0, \quad \boldsymbol{x} \in \Gamma_D^u, \\ -k\frac{\partial\theta}{\partial n} &= 0, \quad \boldsymbol{x} \in \Gamma_N^T, \quad \theta = \theta_0, \quad \boldsymbol{x} \in \Gamma_D^T, \end{aligned}$$

where $\partial\Omega = \Gamma_D^u + \Gamma_N^u = \Gamma_D^\theta + \Gamma_R^\theta$.

3 Approximation by Space

For numerical solution, we rewrite Eqs. (1) and (2) in weak form, using integration by parts to eliminate second derivatives [5–10].

Let $H = L_2\,(\Omega)$ be the Hilbert space for temperature increment with following scalar product and norm:

$$(u, v) = \int_\Omega u(\boldsymbol{x})\,v(\boldsymbol{x})\,dx, \quad ||u|| = (u, u)^{1/2},$$

and $\boldsymbol{H} = (L_2\,(\Omega))^d$ be space for displacement, where $\Omega \in \mathbb{R}^d$, $d = 2, 3$.

Then letting test functions q and $\boldsymbol{v}$ vanish on the appropriate Dirichlet boundaries Γ_D^θ and $\Gamma_D^{\boldsymbol{u}}$, respectively, where solutions are known, we receive following variational problem: find $\theta \in V_\theta$ and $\boldsymbol{u} \in \boldsymbol{V_u}$ such that

$$\textstyle\int_\Omega (k\,\mathrm{grad}\,\theta,\,\mathrm{grad}\,q)dx + \int_\Omega f\,q\,dx \quad \forall q \in \hat{V}_\theta = 0, \tag{3}$$

$$\int_\Omega \boldsymbol{\sigma}(\boldsymbol{u})\,\boldsymbol{\varepsilon}(\boldsymbol{v})dx + \int_\Omega \alpha(\operatorname{grad}\theta, \boldsymbol{v})dx = 0 \quad \forall \boldsymbol{v} \in \hat{\boldsymbol{V}}_{\boldsymbol{u}}, \tag{4}$$

where test spaces $\hat{V}_\theta$ and $\hat{\boldsymbol{V}}_{\boldsymbol{u}}$ are defined by

$$\hat{V}_\theta = \{q \in H^1(\Omega) : q(\boldsymbol{x}) = 0, \quad \boldsymbol{x} \in \Gamma_D^\theta\},$$

$$\hat{\boldsymbol{V}}_{\boldsymbol{u}} = \{\boldsymbol{v} \in H^d(\Omega) : \boldsymbol{v}(\boldsymbol{x}) = 0, \quad \boldsymbol{x} \in \Gamma_D^{\boldsymbol{u}}\},$$

and the trial spaces V_θ and $\boldsymbol{V}_{\boldsymbol{u}}$ are shifted from test spaces by the Dirichlet boundary conditions:

$$\hat{V}_\theta = \{q \in H^1(\Omega) : q(\boldsymbol{x}) = \theta_0, \quad \boldsymbol{x} \in \Gamma_D^\theta\},$$

$$\hat{\boldsymbol{V}}_{\boldsymbol{u}} = \{\boldsymbol{v} \in H^d(\Omega) : \boldsymbol{v}(\boldsymbol{x}) = \boldsymbol{u}_0, \quad \boldsymbol{x} \in \Gamma_D^{\boldsymbol{u}}\}.$$

Further, we define the following bilinear and linear forms on the defined spaces

$$b(\theta, q) = \int_\Omega (k \operatorname{grad}\theta, \operatorname{grad} q)dx, \quad l(q) = (f, q) = \int_\Omega f\, q\, dx,$$
$$a(\boldsymbol{u}, \boldsymbol{v}) = \int_\Omega \boldsymbol{\sigma}(\boldsymbol{u})\,\boldsymbol{\varepsilon}(\boldsymbol{v})dx, \quad g(\theta, \boldsymbol{v}) = \int_\Omega \alpha(\operatorname{grad}\theta, \boldsymbol{v})dx.$$

Then problem becomes: find $\theta \in V_\theta$ and $\boldsymbol{u} \in \boldsymbol{V}_u$ that satisfy the following relations

$$b(\theta, q) + l(q) = 0 \quad \forall q \in \hat{V}_\theta, \tag{5}$$

$$a(\boldsymbol{u}, \boldsymbol{v}) + g(\theta, \boldsymbol{v}) = 0 \quad \forall \boldsymbol{v} \in \hat{\boldsymbol{V}}_u. \tag{6}$$

Note that these parts of problem are solved successively. First, we find distribution of temperature field from (5). And then we use it for calculation of displacement in (6).

4 Numerical Results

The object of research is ceramic substrates with metallization, which are used for the manufacturing of LED modules. During the creation process these substrates are subjected to significant heating, thereby an elastically-stressed state occurs, which leads to cracking of the substrate in some cases.

One of the ways of improvement is the minimization of the elastic stresses in the ceramic substrate with metallization. To find solution of this problem we need calculate elastic stress state of ceramic substrates under the influence of thermal stress raises.

The substrate has the length of 130 mm, the width of 72 mm and the thickness of 0.635 mm and 0.03 mm for ceramic and metal layers, respectively. On both sides it has technological holes of 1 mm and 1.5 mm diameter. Also the ceramic side has deepening of 0.2 mm with width of 0.1 mm. The full geometry of the object is shown in Fig. 1.

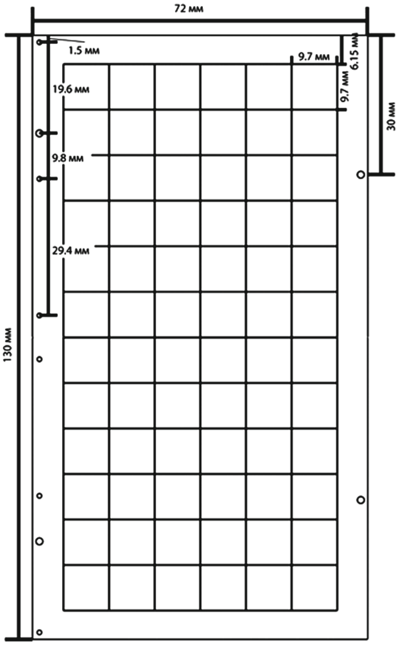

Fig. 1. Ceramic substrate geometry

To verify the model with the experimental data we use the temperature distribution along the middle line of the substrate. The boundary conditions for heating and cooling the substrate are modeled by appropriate Robin boundary conditions corresponding to convection with ambient air and metal rails. In this case the heat flux is modeled as convection with strongly heated air. These boundary conditions can be represented as following equations:

$$k \frac{\partial \theta}{\partial n} = \beta_i (\theta - \theta_i), \quad x \in \Gamma_i, \quad i = 1, 2, 3, 4, \tag{7}$$

where k is coefficient of thermal conductivity, β_i is heat transfer coefficient with air when $i = 1, 4$ and with metal when $i = 2, 3$, θ_i is difference between

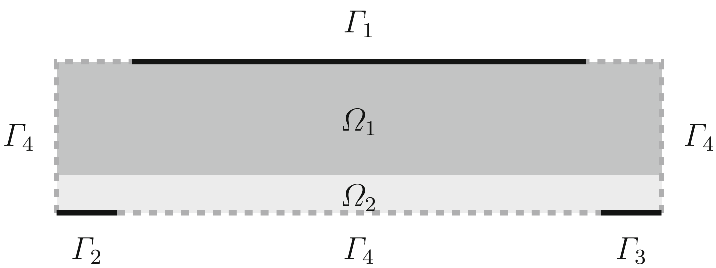

Fig. 2. Boundaries and domains in a slice

temperature of i-th boundary and initial temperature of substrate. Respective boundaries of heat flux Γ_1, convection with rails Γ_2, Γ_3 and air Γ_4, also ceramic layer Ω_1 and metal layer Ω_2 domains represented in Fig. 2.

For the following values: $k = 20\mathrm{W/(m\cdot K)}$ for ceramic and $k = 400\mathrm{W/(m\cdot K)}$ for metallization, $\beta_{1,4} = 5\mathrm{W/(m^2\cdot K)}$, $\beta_{2,3} = 400\mathrm{W/(m^2\cdot K)}$, $\theta_1 = 270C^0$, $\theta_2 = 90C^0$, $\theta_3 = 75C^0$ and $\theta_4 = 95C^0$, temperature distribution along the midline was obtained, which agrees with field experiments. In Fig. 3 a comparison of the temperature along the midline for the model and experiment is shown.

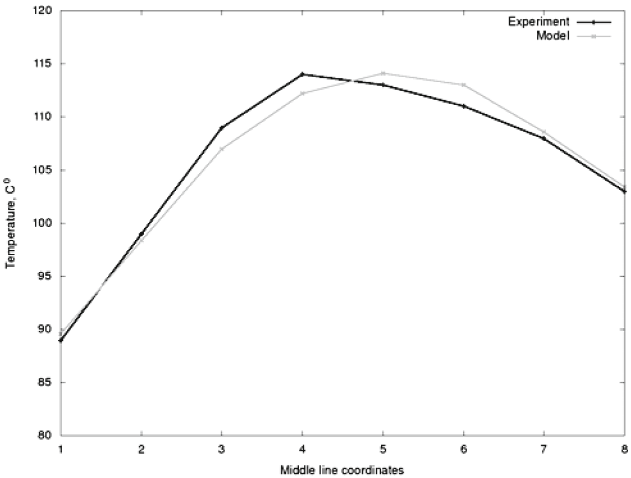

Fig. 3. Temperature distribution along the middle line (experiment, model)

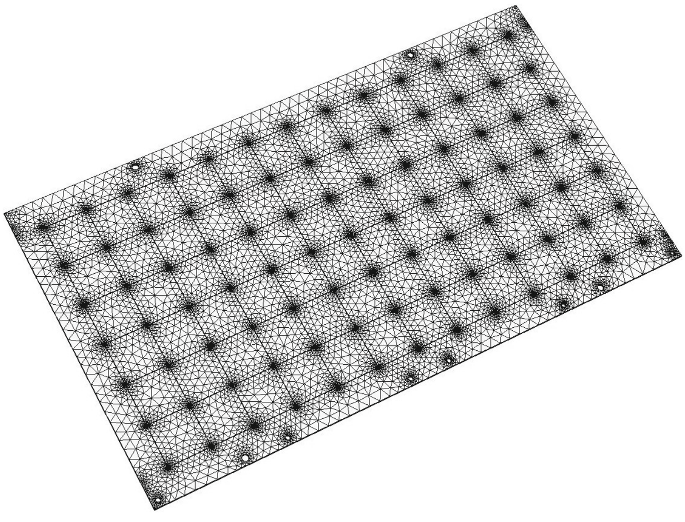

Fig. 4. Computational domain

In this work the simulation is performed using the first-degree polynomial approximation for temperature and first-degree for displacement. To solve the arising system of linear equations a standard direct method of ILU-factorization is used. A collection of free software FEniCS [11] is used for the numerical solution, and open-source application Paraview is used for visualization of the results.

For numerical modeling of thermoelasticity problem for ceramic substrate with metallization three grids containing about 250 000, 450 000 and 1 000 000 cells are used. These grids were made in Netgen mesh generator program. As for example, the finest grid with more than million cells is shown in Fig. 4. As results of numerical computation temperature distribution across the substrate (Fig. 5) and von Mizes stress distribution in technological hole (Fig. 6) are presented.

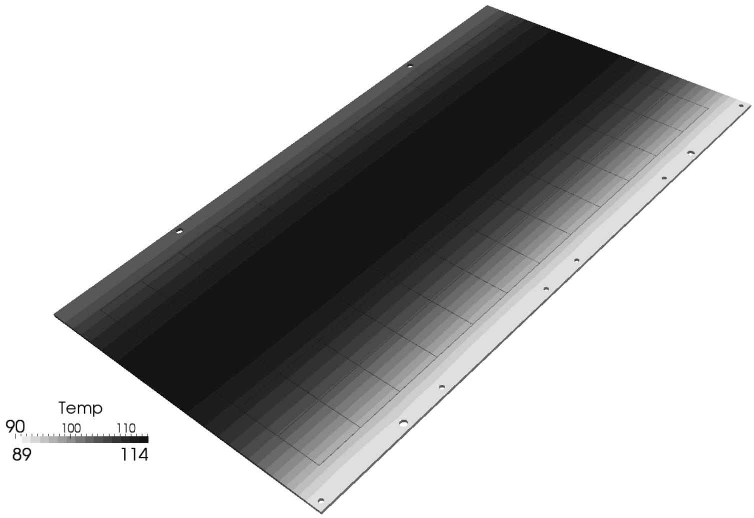

Fig. 5. Temperature distribution

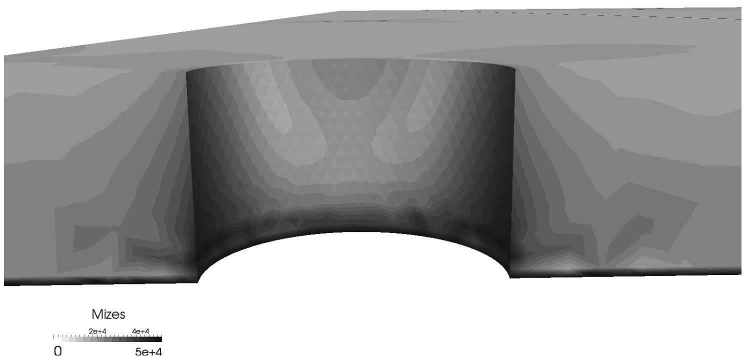

Fig. 6. Mizes stress distribution in technological hole

Table 1. Dependence of computation time (in seconds) from number of processes for different grids

Grid size	Number of processes					
	1	2	4	8	16	32
250 000	119	87	53	44	49	53
450 000	199	133	87	70	78	86
1 000 000	433	347	206	181	161	160

To illustrate the effectiveness of parallelization on a cluster, a series of computational experiments on three grids with different amounts of running processes are made. The results of gained dependence of computation time from number of processes are given in Table 1.

Table 1 shows the effectiveness of parallelization on different amount of running processes. Note that the effectiveness is evident for all presented grids. Moreover, for each grid we have optimal number of running processes. For instance, the first and second grids have the fastest computation when 8 processes are used. And for the third grid it is optimal to use 16 processes, as further growth of the computational resources does not gain any acceleration.

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