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# NUMERICAL MODELING OF THERMOMECHANICAL STRESSES GENERATED IN A THIN FILM UNDER LASER-PULSE ACTION

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**Abstract**

We develop a mathematical model for calculating thermomechanical stresses generated in a thin film under laser-pulse action. We propose a model that also allows one to evaluate the duration of transient processes and determine laser-pulse parameters, including a profile that is particularly useful for studies of triboluminescent materials. The model includes a nonstationary heat equation and a thermoelasticity equation, which we solve numerically using the finite difference method.

**Keywords:** mathematical model, thermoelasticity equation, heat equation, mechanical stress.

## 1. Introduction

Triboluminescence is a visible or infrared light generated under the action of mechanical forces, such as static, dynamic, or pulsing fields of pressure or deformations [1]. Triboluminescent (TL) materials are of great interest to engineers as promising materials for external tactile signal sensors in robotics and new nondestructive control methods [2–5].

In [2], a mathematical model was developed for evaluating the triboluminescent light flux for known deformation stresses in materials. But in the experiments with TL materials, where luminescence arises due to the action of short ($10^{-6} - 10^{-3}$ s) laser pulses with small radii of the laser beams, the stress values cannot be obtained directly from the experiment [6,7]. Therefore, the elaboration of mathematical models for determining mechanical stresses in materials with account of the laser-pulse parameters is of crucial interest.

The mathematical model under consideration is applied to a thin film on a massive substrate under the action of a temperature field in the approximation of ideal film–substrate adhesion and short laser pulse. According to [8], we may neglect the influence of the substrate heat properties on the film heating process.

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## 2. Mathematical Model

The problem can be mathematically modeled by a system of equations that includes the heat equation [9] describing a nonstationary laser-generated temperature field in the film and the thermoelasticity equations [10] describing mechanical stresses generated by heating of the film,

$$\begin{cases} \rho c \dfrac{\partial T}{\partial t} - A\nabla(\lambda_q \nabla T) = f(x,y,z) = 0, \\ \nabla^2(\sigma_{xx}+\sigma_{yy}) + E\alpha_T \nabla^2(T-T_0) = 0, \\ \dfrac{\partial \sigma_{xx}}{\partial x} + \dfrac{\partial \sigma_{xy}}{\partial y} = 0\,, \qquad \dfrac{\partial \sigma_{xy}}{\partial x} + \dfrac{\partial \sigma_{yy}}{\partial y} = 0\,, \end{cases} \tag{1}$$

where $\rho$ is the material density, $c$ is the specific heat, $A$ is the absorption efficiency of the film, $\lambda_q$ is the thermal conductivity, $T$ is the temperature, $t$ is the time, $x$, $y$, and $z$ are the space coordinates, $f(x,y,z)$ is the density of the heat-source field, $E$ is the Young modulus, $\alpha_T$ is a linear thermal expansion coefficient, $\sigma_{xx}$, $\sigma_{xy}$, and $\sigma_{yy}$ are the stress tensor components, and $T_0$ is the initial temperature of the material.

A peculiarity of the system of equations (1) consists of the combination of the first- and second-order differential equations. In approximating (1), we cannot use forward or backward differences in the first-order equations, since it breaks the symmetry of the solution, and therefore inadequate results are obtained. We cannot use the central differences, since they lead to zero values on the main diagonal of the coefficient matrix of the system of linear algebraic equations, providing an approximate solution of (1). In this paper, we avoid this difficulty by differentiating the first-order differential equations to obtain the second-order equations as follows:

$$\frac{\partial^2 \sigma_{xx}}{\partial x^2} + \frac{\partial^2 \sigma_{xy}}{\partial x \partial y} = 0, \qquad \frac{\partial \sigma_{xy}}{\partial x \partial y} + \frac{\partial^2 \sigma_{yy}}{\partial y^2} = 0, \qquad \frac{\partial^2 \sigma_{xx}}{\partial x^2} - \frac{\partial^2 \sigma_{yy}}{\partial y^2} = 0, \tag{2}$$

$$\frac{\partial^2 \sigma_{xx}}{\partial x \partial y} + \frac{\partial^2 \sigma_{xy}}{\partial y^2} = 0, \qquad \frac{\partial^2 \sigma_{xy}}{\partial x^2} + \frac{\partial^2 \sigma_{yy}}{\partial x \partial y} = 0, \qquad \frac{\partial^2 \sigma_{xy}}{\partial x^2} + \frac{\partial^2 \sigma_{xy}}{\partial y^2} = -\frac{\partial^2 \sigma_{xx}}{\partial x \partial y} - \frac{\partial^2 \sigma_{yy}}{\partial x \partial y}. \tag{3}$$

Taking into account (2) and (3), we can transform the system of equations (1) and arrive at

$$\begin{gathered} \rho c \frac{\partial T}{\partial t} - A\nabla(\lambda_q \nabla T) = 0, \qquad \nabla^2(\sigma_{xx}+\sigma_{yy}) + E\alpha_T \nabla^2(T-T_0) = 0, \\ \frac{\partial^2 \sigma_{xx}}{\partial x^2} - \frac{\partial^2 \sigma_{yy}}{\partial y^2} = 0, \qquad \nabla^2 \sigma_{xy} = -\frac{\partial^2 \sigma_{xx}}{\partial x \partial y} - \frac{\partial^2 \sigma_{yy}}{\partial x \partial y}. \end{gathered} \tag{4}$$

We chose the initial conditions for the heat equation (1) as

$$T(x,y,z,t_{\min}) = T_0(x,y,z), \tag{5}$$

where $t_{\min}$ is the initial time, and $T_0(x,y,z)$ is the initial temperature distribution at time $t_{\min}$.

To transform the first-order equation in a second-order equation, we need additional boundary conditions, which we take as follows:

$$T(x,y,z_{\max}) = T_0(x,y,z_{\max}), \qquad T(x,y_{\min},z) = T_0(x,y_{\min},z), \qquad T(x,y_{\max},z) = T_0(x,y_{\max},z),$$
$$T(x_{\min},y,z) = T_0(x_{\min},y,z), \qquad T(x_{\max},y,z) = T_0(x_{\max},y,z), \tag{6}$$

$$\left.\frac{\partial T}{\partial z}\right|_{\substack{x^2+y^2>D^2/4\\ z=z_{\min}}} = 0, \qquad \left.\frac{\partial T}{\partial z}\right|_{\substack{x^2+y^2\le D^2/4\\ z=z_{\min}}} = -4E_L/(\pi D^2\tau\lambda_q)\exp\left[-8(x^2+y^2)/D^2\right], \tag{7}$$

$$\begin{aligned}
&\sigma_{xx}(x,y_{\min}) = \sigma_{xx}(x,y_{\max}) = \sigma_{xx}(x_{\min},y) = \sigma_{xx}(x_{\max},y) = 0,\\
&\sigma_{yy}(x,y_{\min}) = \sigma_{yy}(x,y_{\max}) = \sigma_{yy}(x_{\min},y) = \sigma_{yy}(x_{\max},y) = 0,\\
&\sigma_{xy}(x,y_{\min}) = \sigma_{xy}(x,y_{\max}) = \sigma_{xy}(x_{\min},y) = \sigma_{xy}(x_{\max},y) = 0,
\end{aligned} \tag{8}$$

where $x_{\min}$, $x_{\max}$, $y_{\min}$, and $y_{\max}$ are the area boundaries, $z_{\min}$ is the coordinate of the top (laser-heated) film boundary, $z_{\max}$ is the coordinate of the bottom (film–substrate) film boundary, $D$ is the laser-beam patch diameter on the film surface, $E_L$ is the laser pulse energy, and $\tau$ is the laser pulse duration.

We employ the boundary conditions (6)–(8) taking into account the following approximations:

- The bottom film boundary temperature is constant and equals the substrate temperature (6);
- During the transient process considered in the problem, the temperatures of the side boundaries are constant (7);
- Energy losses due to heat transfer from the top film surface, other than the laser beam patch, are neglected (8);
- The heat flux on the top film surface in the laser-beam patch area (with diameter $D$) is set according to the laser-pulse energy and duration (8). The right-hand side of (8) shows the laser-beam-power distribution in space (here, the Gaussian profile [11]);
- There are no mechanical stresses at the side boundaries of the film (8), and this fact adds some restrictions on the minimum size $(x-y)$ of the film area under consideration.

In the general case, the heat transfer and thermoelasticity problems must be solved in 3D, but if we consider a thin film on a massive substrate, we can solve the thermoelasticity problem in 2D ($x$ and $y$) only. Combining these 2D and 3D equations, we transform the 3D nonstationary temperature distribution to the 2D distribution using the expression

$$T(x,y,t) = \max\left[T(x,y,z,t)\right]. \tag{9}$$

We need to obtain the 3D numerical solution of the heat transfer equation, because for the 2D heat transfer equation the laser-beam-energy flux on the surface should be approximated by an equivalent internal energy source, and that is not correct.

## 3. Results of Numerical Modeling

To solve the system of equations (4)–(8), using the finite difference method, we developed a numerical code pack [12], which enables us to obtain temperature fields and mechanical stress tensor components

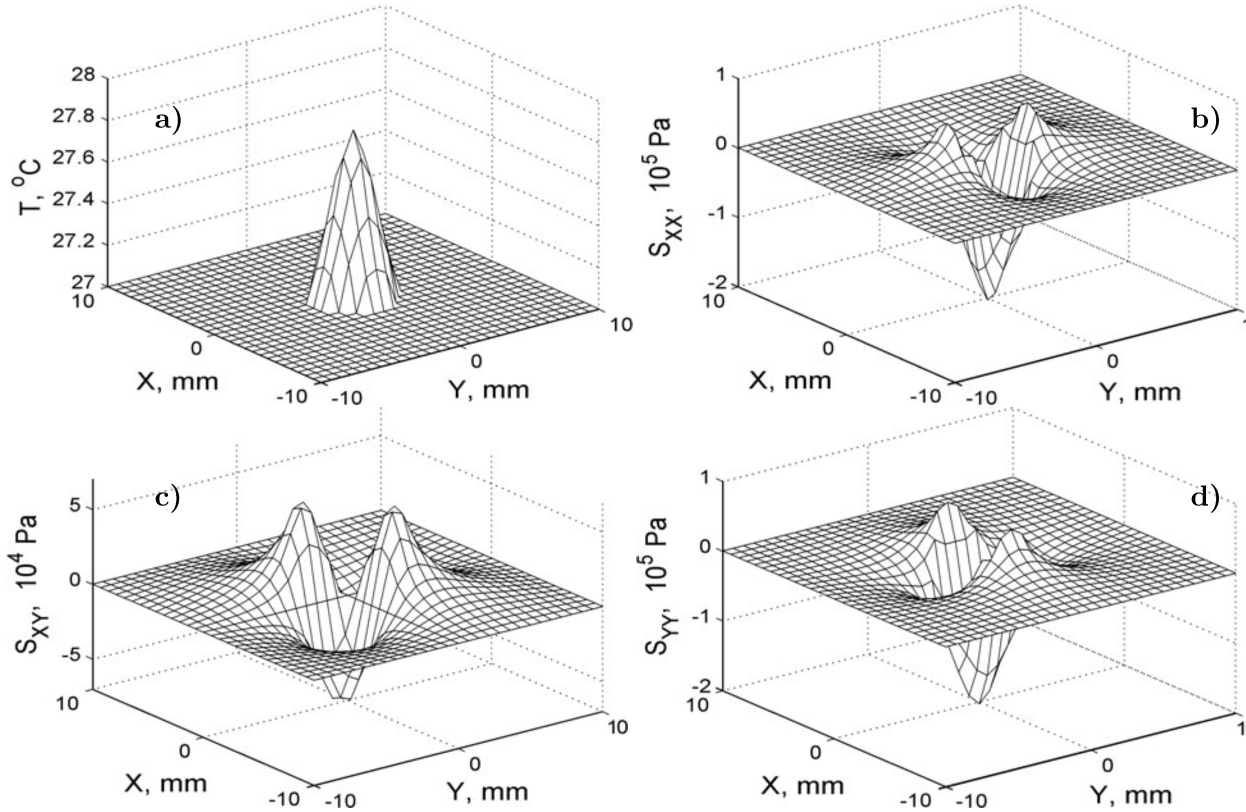


**Fig. 1.** Temperature field (a) and stress-tensor component $\sigma_{xx}$ (b), $\sigma_{xy}$ (c), and $\sigma_{yy}$ (d) distributions on the ZnS (TL) film surface (10 $\mu$m thick) at time $t = 2.5$ $\mu$s at the end of the laser pulse. The laser pulse has a rectangular time profile and a Gaussian power-distribution profile across the beam (average power density 283 W/mm$^2$ and duration 9 $\mu$s) and is focused on a patch of radius 2.5 mm.

for any given distribution of the laser-beam power in time and space. Figures 1–3 show the results of numerical modeling of the laser-beam action on the zinc sulfate (ZnS) triboluminescent film (thermal and mechanical parameters are shown in Table 1 [13]). We solved the problem in the approximation of constant elastic and thermal expansion coefficients.

**Table 1.** Thermal and Mechanical Parameters of ZnS [13].

| Parameter | Value |
|---|---|
| Density, $\rho$ | 4090 kg·m$^{-3}$ |
| Specific heat, $c$ | 124 J/kg·K |
| Thermal conductivity, $\lambda_q$ | 27.2 W/m·K |
| Young modulus, $E$ | $7.4 \cdot 10^{10}$ Pa |
| Linear thermal expansion coefficient, $\alpha_T$ | $6.8 \cdot 10^{-6}$ K$^{-1}$ |

Figure 1 shows the temperature and stress-tensor components $\sigma_{xx}$, $\sigma_{xy}$, and $\sigma_{yy}$ of the fields on the surface of the ZnS triboluminescent film (10 $\mu$m thick) at the end of the laser pulse. The laser pulse has

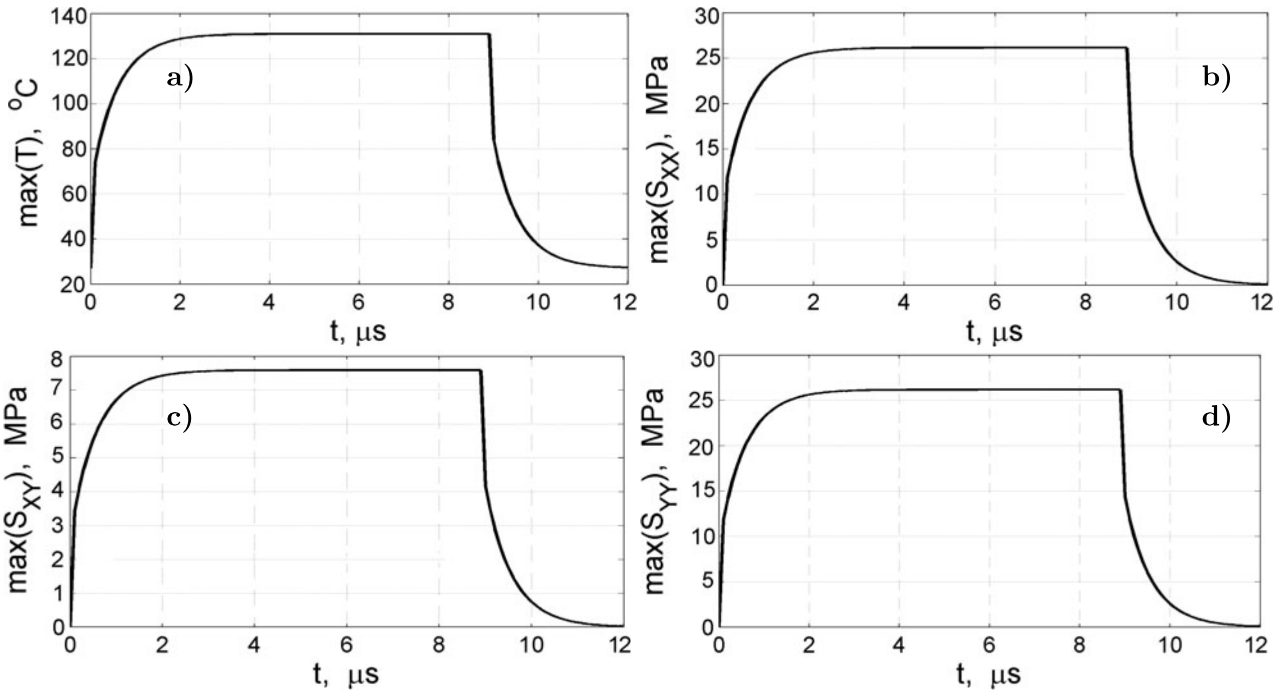


**Fig. 2.** Time dependences of the maximum temperatures (a) and stress-tensor components $\sigma_{xx}$ (b), $\sigma_{xy}$ (c), and $\sigma_{yy}$ (d) on the ZnS (TL) film surface for the same laser pulse as in Fig. 1.

a rectangular time profile, a Gaussian power-distribution profile across the beam (average power density 283 W/mm$^2$ and duration 9 $\mu$s), and is focused on a patch of radius 2.5 mm.

In Fig. 2, we show the time dependences of the maximum temperatures and the stress-tensor components on the surface of the ZnS (TL) film for the same laser pulse.

Fast increase and decrease in the maximum temperature on the film surface (see Fig. 2) follow from the high-power density of the laser pulse (283 W/mm$^2$) accompanied at the same time by relatively high inertia of the heat transfer in the film. Moreover, we did not take into account the heat losses from the film surface, which is an acceptable assumption for such small laser-pulse duration [9]. Also we assume a full absorption of the laser pulse energy in the film material in our model. Other mechanisms of the energy dissipation can be added employing the film absorption efficiency $A$ available in the model.

Figure 3 shows the dependences of the duration of transient processes $T_{\rm tr}$ on the film specific heat, thermal conductivity, and thickness. To estimate the duration of transient processes $T_{\rm tr}$, we calculated the maximum temperature and mechanical stress-tensor components in the film. As the duration of the transient processes, we assume the time when the considered values enter the 10% range from the long-time established value.

The results presented in Figs. 2 and 3 allow us to evaluate the duration of transient processes for the case where the temperature and mechanical stress-tensor components are changed. These evaluations for materials with different heat parameters and films of different thickness allow one to obtain the dependence of the TL light intensity observed in experiments on the unobservable mechanical stress-tensor values for given parameters of the laser pulse.

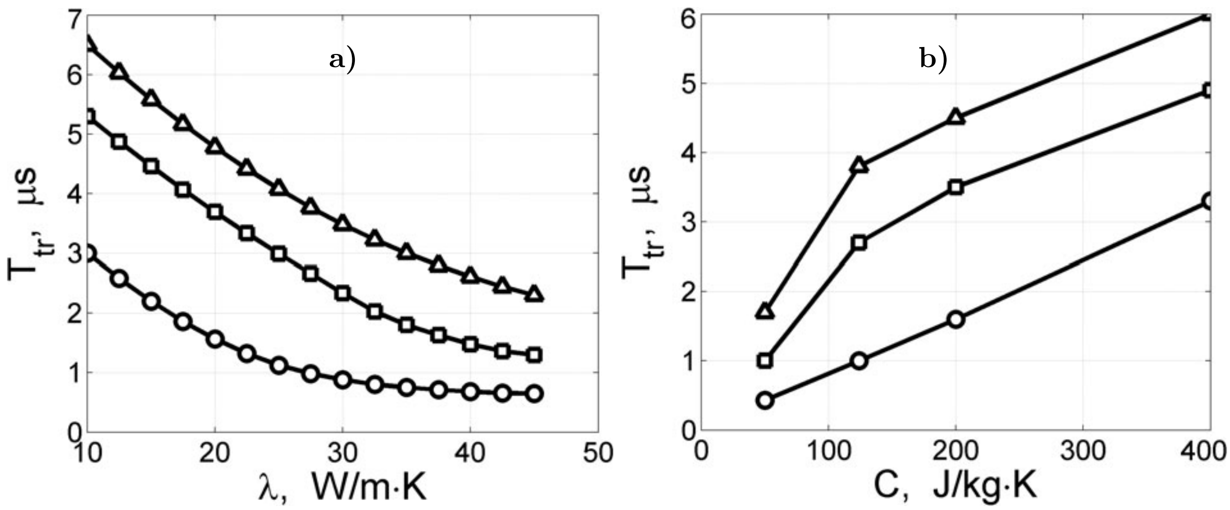


**Fig. 3.** Dependences of the duration of transient processes on the thermal conductivity $\lambda_q$ (a) and specific heat (b) at a film thickness $h$ of 10 (○), 15 (□), and 20 $\mu$m(△).

## 4. Conclusions

The mathematical model we proposed [Eqs. (4)–(8)] and the numerical code pack developed [12] allow us to calculate the temperature and mechanical stress-tensor component distributions in space and time in triboluminescent films.

Analysis of the calculated values provides

- The dependence of the maximum temperature and stress-tensor components $\sigma_{xx}$, $\sigma_{xy}$, and $\sigma_{yy}$ on the laser pulse parameters;
- Parameters of the transient processes, including their durations;
- Parameters and profile of the laser pulse used for generating needed stresses and temperatures in the films, which are useful for studying the TL materials.

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