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Mechanism of laser damage of transparent semiconductors

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Abstract

Damage of transparent semiconductors and dielectrics under the action of high-intensity laser radiation fluxes is mainly attributed to absorptive inclusions, which being heated up to the melting threshold, result in thermal stresses due to the occurrence of microcracks and pores in materials. In this connection a local spherical area molten by laser radiation and then solidifying in a transparent solid in conditions of external cooling is considered and the temperature fields in the solidified region are calculated. The temperature fields and temporary stress dependences on thickness of a solidified region at different speeds of a solidified front are graphically analyzed. The conditions of occurrence of caverns in irradiated crystals are discussed. The present results can be used in the analysis of the damage processes of optical components of power laser devices, in particular made from ZnSe semiconductors.

Keywords: Stress simulation; Temperature field; Laser irradiation; ZnSe crystals

1. Introduction

Interacting with transparent semiconductors high-intensity laser radiation fluxes usually result in local heating of inhomogeneities in the bulk up to the melting point of the material [1]. This has been attributed to the presence of light-absorptive macroinclusions and micro-inclusions with dimension of the order of wavelength in the crystals. In the last case these inhomogeneities are heated in a recombination mechanism [2]. It was shown [3] that there is also an own mechanism of nucleation of an elementary defect related to accumulating light energy in a thermal fluctuation of density (tensile strain) resulting in the formation of a stable germinal crack. Nevertheless, in all cases laser irradiation of transparent materials with an intensity close to a melting threshold results in heating, melting and subsequent solidifying of local areas in the bulk of a solid. In particular, it is related to short laser pulses of nano- and femtosecond duration [4]. Fast crystallization of a laser-melted area in a crystal forms elastically deformed regions that can cause the occurrence of microcracks and caverns in materials. It was shown that the irradiation of highly pure, specially undoped, ZnSe single crystals with nanosecond ruby laser pulses can result in both tensile and compressive strain [5,6] as well as in increase of optical absorption in the transparency range of the semiconductor [7]. In the present paper the model of a local spherical area molten by laser radiation and then solidifying in a transparent solid in conditions of external cooling is considered according to the approach reported in Ref. [8]. The stresses and temperature fields in the local solidified region of the bulk of a transparent solid are determined.

2. Definition of the state of solidifying sphere

2.1. The strained state of elastic solid sphere with radial temperature distribution

We consider a hollow sphere with spherically symmetrical distribution of temperature $T(r)$. R is the external radius of a sphere, r_0 is the internal radius. The state of an elastically deformed solid is featured by the strain

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vector $\boldsymbol{U}$, strain tensor U_{ik} and stress tensor σ_{ik} [9]. The equilibrium equation for a deformed solid is

$$\frac{\partial \sigma_{ik}}{\partial x_k} = 0, \quad i,k = 1,2,3. \tag{1}$$

The relation between strain tensor and stress tensor, which characterizes an elastic medium, is expressed by the Hook law

$$\sigma_{ik} = 2\mu U_{ik} + \left(K - \frac{2}{3}\mu\right) U_{jj}\delta_{ik} - 3K\alpha(T - T_0)\delta_{ik}, \tag{2}$$

where T_0 is the equilibrium temperature. The last item of this expression represents the stresses which are due to a temperature variation of a body. Here α is the linear expansion coefficient, μ is the shear modulus and K is the compression modulus for an elastic body. These values are regarded as constants. Solving Eqs. (1) and (2) in the spatial polar coordinates (r, φ, θ) and using boundary conditions that both the external and internal sphere surfaces are stressless $\sigma_{rr}|_{r=r_0} = 0$, $\sigma_{rr}|_{r=R} = 0$, the radial and circular components of the stress tensor can be obtained in a view:

$$\sigma_{rr}(r) = \frac{2\mu 9K}{3K + 4\mu} \times \left[\frac{r^3 - r_0^3}{R^3 - r_0}\frac{2}{r^3}\int_{r_0}^{R} \alpha T(r) r^2\,\mathrm{d}r - \frac{2}{r^3}\int_{r_0}^{r} \alpha T(r) r^2\,\mathrm{d}r\right], \tag{3}$$

$$\sigma_{\varphi\varphi}(r) = \sigma_{\theta\theta}(r) = \frac{2\mu 9K}{3K + 4\mu}\left[\frac{2r^3 + r_0^3}{R^3 - r_0}\frac{1}{r^3} \times \int_{r_0}^{R} \alpha T(r) r^2\,\mathrm{d}r - \frac{1}{r^3}\int_{r_0}^{r} \alpha T(r) r^2\,\mathrm{d}r - \alpha T(r)\right]. \tag{4}$$

2.2. The temperature distribution in solidifying sphere

In a solidifying sphere the temperature field $T(r)$ is related with motion of a solidified front. In order to define the temperature dependence $T(r)$ for Eqs. (3) and (4) it is necessary to consider the problem of temperature distribution in a body with varying boundary, the so-called Stephan problem [10]. The condition on the phase boundary is

$$\frac{Q}{c}\frac{\partial \eta(t)}{\partial t}\bigg|_{r=\eta(t)} = \frac{\partial T}{\partial t}\bigg|_{r=\eta(t)},$$

where Q is the crystallization heat, c is the heat capacity, $\eta(t)$ is the radius of the phase boundary which moves under the law

$$\eta(t) = \sqrt{4wa(t_* - t)}, \tag{5}$$

where w is the dimensionless parameter characterizing the intensity of a heat rejection and thus determining the speed of motion of the phase boundary, $a = \chi/C_\mathrm{v}$ is the thermal diffusivity, χ is the thermal conductivity, C_v is the heat capacity at constant volume, t is the time and t_* is the time during which the crystallization is finished. The initial condition for the solidification boundary is $\eta(0) = 1$ and the second boundary condition requires stationary temperature at a solidified front

$$T(r,t)|_{r=\eta(t)} = T_*,$$

where T_* is the crystallization temperature. Solving the thermal conduction equation [10] for a centrally symmetric temperature field in spatial polar frame while taking into account the initial and boundary conditions above, one can compute the temperature field in a solidifying sphere under external cooling:

$$T(r,t) = \frac{Q}{c}\mathrm{e}^{-w} w^{3/2}\int_{(w(r^2)/\eta^2(t))}^{w} \mathrm{e}^{x} x^{-3/2}\,\mathrm{d}x + T_*. \tag{6}$$

2.3. Definition of temporary stresses in solidifying sphere

We consider a melted sphere with radius $R = 1$. The internal surface of a sphere is a solidified front. The crystallization process is started at $t = 0$ and for $t \geqslant 0$ a position of the crystallization boundary $r = \eta(t)$ is defined by Eq. (5) and the temperature distribution in the solidified region $T(r,t)$ is expressed by Eq. (6). It is guessed that the speed of material elements is small compared to that of a solidified front. In the solidified region the equilibrium equations, Eq. (1), and the Hook law, Eq. (2) are valid. The thickness of the solid region varies during solidification. Thus it is necessary to determine stresses in a body with a variable boundary. It was shown [8] that the description of such problems was convenient to make using variables characterizing an instantaneous state of a solid. Such variables are a vector field of speeds and tensor field of speeds of deformations. Therefore, in order to characterize an instantaneous state of a solid, Eqs. (1) and (2) differentiated with respect to time are used. These expressions are valid for an ideal liquid using the shear modulus $\mu = 0$. $\tilde{K}$ is the compression modulus for a liquid and the pressure p of a melt instead of stresses σ_{ik} is supposed. In this case the change rate of pressure is used as an instantaneous variable.

The joint change of state of both a strained liquid and solid is esteemed. Therefore the conjugation conditions at the boundary between a melt and solid are used. The density at the crystallization boundary undergoes a jump. The conjugation, which is a consequence of the mass conservation law, reflects this fact:

$$\rho\left(v - \frac{\mathrm{d}\eta(t)}{\mathrm{d}t}\right)\bigg|_{r=\eta(t)} = \tilde{\rho}\left(\tilde{v} - \frac{\mathrm{d}\eta(t)}{\mathrm{d}t}\right)\bigg|_{r=\eta(t)}, \tag{7}$$

where ρ, $\tilde{\rho}$ are the densities and v, $\tilde{v}$ are the strain speeds of a solid and melt, respectively. Usually at solidification of a melt there is a shrinkage which is due to the fact that the density of a solid is more than the density of a melt ($\tilde{\rho}/\rho < 1$); therefore, the liquid appears comprehensively tensile ($p(t)|_{t\neq 0} < 0$). In the process of moving a solidified front the tension of a liquid increased. At some value of tension (at the moment of $t = t_c$) the collapse in a liquid occurs with forming a gap and therefore a cavern in a solid. Thus, the pressure inside a sphere drops to the zero point.

On the basis of the discussed model and using the initial, boundary and conjugation conditions, the expressions for the temperature dependences and temporary stresses dependences on thickness of a solidified region at different speeds of a solidified front w (or intensity of a heat rejection) were obtained. Inasmuch as the obtained analytical expressions were very cumbersome, it was possible to expediently analyze them graphically in dimensionless variables, using computer calculation (Figs. 1–4). The dimensionless variables were defined using the radius of a melted sphere $R = 1$ and by dividing the obtained expression on the combination of dimension constants characterizing the material [8]. The ZnSe semiconductor constants were used [11].

3. Analysis of theoretical results

The motion of a solidified front (i.e. an increase in thickness of a solidified region) is represented as a decrease in r in the figures. The two cases of the heat rejection intensity ($w_1 = 0.01$ and $w_2 = 0.02$) are considered. Fig. 1 demonstrates that the temperature field is dependent on the thickness of solidified layer. On moving a solidified front, the temperature on the external surface of a sphere is lowered in the course of time because of the heat to be retracted through a more

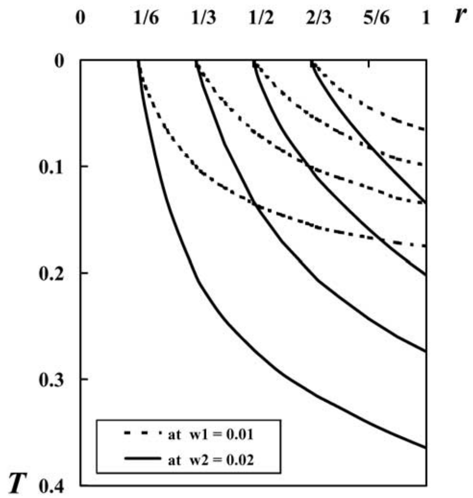

Fig. 1. Temperature distributions $T(r)$ in a solidifying sphere at different thicknesses r of solidified region and at different heat rejection intensities w (solidified front speed).

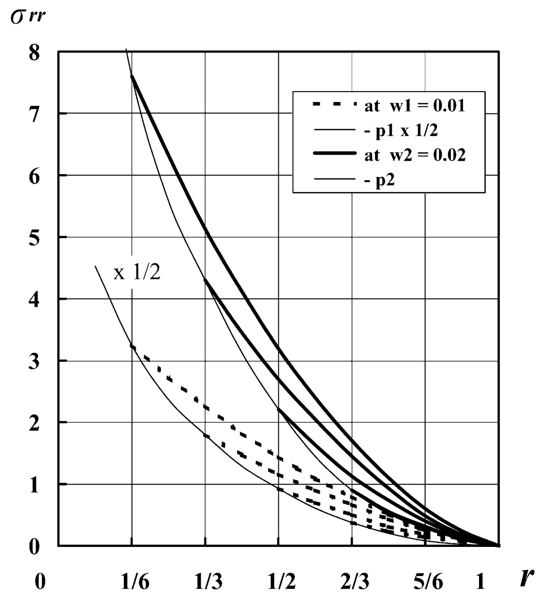

Fig. 2. Radial stresses $\sigma_{rr}(r)$ in a solidifying sphere before forming a cavern at different thicknesses r of solidified region and at different heat rejection intensities w (solidified front speed). Envelopes (thin curves) represent a module of the pressure p of a melt.

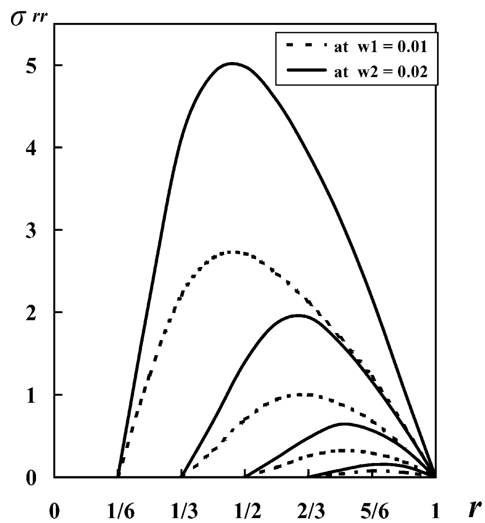

Fig. 3. Radial stresses $\sigma_{rr}(r)$ in a solidifying sphere after forming a cavern at different thicknesses r of solidified region and at different heat rejection intensities w (solidified front speed).

and more thick layer of a rising solid. When the gap in a liquid was not derived yet, the radial stresses have the greatest values on a solidification boundary and numerically are equal to the pressure of a melt (envelopes, i.e. thin curves p_1 and p_2 in Fig. 2) which

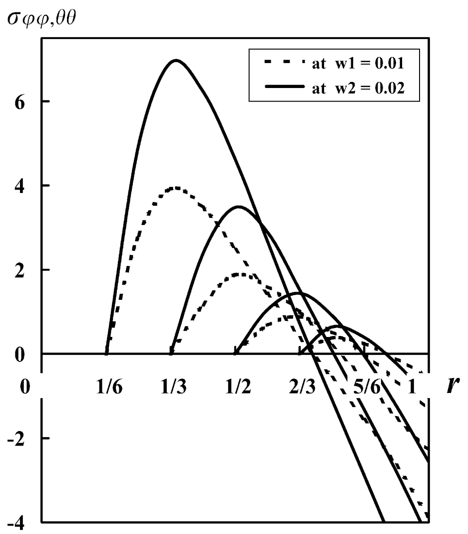

Fig. 4. Circular stresses $\sigma_{\varphi\varphi,\,\theta\theta}(r)$ in a solidifying sphere after forming a cavern at different thicknesses of solidified region r and at different heat rejection intensities w (solidified front speed).

sharply increases with moving a solidified front. After formation of a cavern the maximum of radial stresses is shifted to a solidification boundary on moving a solidified front (i.e. toward smaller r in Fig. 3). The circular stresses have negative values at large radius (Fig. 4) that is an evidence of the formation of tensile strained areas in a solid. The difference in the quantitative nature of the stresses is due to the dependence of the temperature on w in a solidifying body. A rise of w results in an increase in the heat rejection intensity (Fig. 1). The intensive cooling of a body (i.e. an increase in w) results in an increase of the stresses. The stresses also increase on raising the thickness of a crystallized region (Figs. 2–4).

The formation of elastically deformed regions could be the reason for the modification of the photoconductivity spectra of ZnSe crystals [5,6] under irradiation with nanosecond ruby laser pulses. In particular, a shift of the maximum and the red edge of the spectrum toward lower energies can be attributed to the formation of deformed regions with residual stresses (tensile strains) in irradiated crystals. The formation of these regions with a smaller bandgap in irradiated samples conformed with the positive pressure coefficient of the change of the bandgap $dE_g/dp = 6\times10^{-9}$ eV Pa^{-1} for ZnSe [11]. The formation of caverns in local solidified areas of crystals after power laser irradiation (in particular at absorptive inclusions) could cause a rise of the optical absorption in the transparency range of the semiconductor [7].

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