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CALCULATION OF PHASE TRANSITION DYNAMICS UPON LASER IRRADIATION OF SEMICONDUCTORS

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UDC 621.536.592

Approximate expressions are obtained for calculations of the time characteristics of fusion and recrystallization, recrystallization rate, and depth to which the material fuses upon laser annealing of semiconductors. The expressions obtained may be used for selection of processing regimes.

Impulsive processing of semiconductor materials by laser radiation has recently come to be employed in a number of technological applications [1].

Since the fundamental processes which occur in such a situation are assumed to be rapid fusion of a surface layer of the semiconductor and subsequent recrystallization, in order to monitor the phenomena of defect removal, redistributions, and segregation of impurity atoms, and ultimately, the electrophysical properties of this layer, it is necessary to evaluate the parameters of the phase transition: time characteristics of fusion and recrystallization, recrystallization rate, and the depth to which the material fuses. Determination of these parameters experimentally or by numerical methods for solving the thermal conductivity equation using a computer is quite complex and cumbersome.

When the optical radiation absorption coefficients of the material are high, [2, 3] indicated the possibility of calculating these quantities with approximate expressions obtained from time-dependent thermal balance equations using scaling coefficients for more accurate matching of calculated values with those obtained by numerical methods and experimentally.

The present study will utilize a numerical solution of the thermal conductivity equation with consideration of phase transitions and temperature dependence of optical and thermophysical properties to study approximate expressions for the evaluation of laser annealing parameters in a number of semiconductor materials.

It will be assumed that the optical energy is instantaneously transferred to the specimen lattice in the form of heat and is then redistributed through the material by thermal conductivity. Diffusion of hot charge carriers will not be considered.

A one-dimensional thermal flux will be considered, i.e., the dimensions of the irradiated region will be assumed significantly larger than the effective penetration depth of heat into the specimen: $d \gg (2\lambda\tau/\rho c)^{1/2}$, where τ is the time interval over which the phase transitions are accomplished.

With consideration of the above assumptions, we write the thermal conductivity equation

$$c\rho \frac{\partial t}{\partial \tau} = q(x,\ \tau) + \frac{\partial}{\partial x}\left(\lambda(t)\frac{\partial t}{\partial x}\right). \tag{1}$$

Lvov Polytechnic Institute. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 49, No. 1, pp. 132-136, July, 1985. Original article submitted January 30, 1984.

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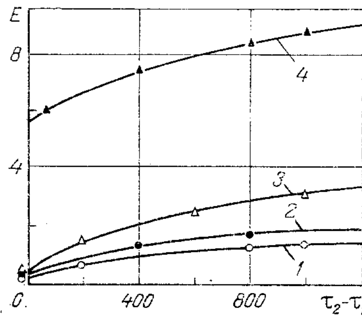

Fig. 1. Change in calculated duration of surface fusion $\tau_2-\tau_1$ (nsec) vs energy density in laser impulse E ($J \cdot cm^{-2}$) (curves): 1) gallium arsenide; 2) germanium; 3) silicon (laser wavelength 0.53 μm); 4) silicon (laser wavelength 1.06 μm, calculation with Eq. (12)); points; experimental data of [4].

The heat source in Eq. (1) is

$$q(x,\ \tau) = \alpha (1 - R) I(\tau) \exp(-\alpha x). \tag{2}$$

We assume that the laser pulse has the form of an isosceles triangle in time:

$$\frac{I(\tau)}{I_{\max}} = \begin{cases} \tau\tau_i^{-1}, & 0 \leqslant \tau \leqslant \tau_i, \\ (2\tau_i - \tau)\tau_i^{-1}, & \tau_i \leqslant \tau \leqslant 2\tau_i, \\ 0, & \tau > 2\tau_i, \end{cases} \tag{3}$$

where the maximum power density is related to the energy density of the laser radiation pulse incident on the specimen $I_{max} = E\tau_L^{-1}$.

Initial and boundary conditions are taken as follows: $t = t_0 = 300°K$ for all x at $\tau = 0$ and $t = t_0$ for all τ at x such that $x > (2\lambda\tau/\rho c)^{1/2}$. During fusion it is assumed that the condition

$$\lambda_s \frac{\partial t}{\partial x} - \lambda_r \frac{\partial t}{\partial x} = \rho H \frac{dx}{d\tau} \tag{4}$$

is satisfied on the moving phase boundary, where $dx/d\tau$ is the fusion or recrystallization rate.

Numerical calculations show that the time at which fusion of the specimen surface commences τ_1 is close to τ_i and decreases, approaching the impulse switch-on time with increase in pulse energy; the time required for fusion of the specimen to the maximum depth L_{max} is greater than the time at which maximum surface temperature t_{max} is attained, while $\tau_L \approx 2\tau_i$ increasing insignificantly with increase in pulse energy, and $\tau_t \approx \sqrt{2}\tau_i$.

From the thermal balance equation for the time $\tau = 2\tau_i$,

$$(1 - R_0) E = c\rho (t_f - t_0)(2\lambda_0\tau/\rho c)^{1/2} \tag{5}$$

an approximate expression was obtained for the minimum energy density in the laser impulse which will produce fusion of the specimen surface:

$$E_{\min} = \left[\frac{4\lambda_0 \rho c \tau_i (t_f - t_0)^2}{\beta_1^2 (1 - R_0)^2}\right]^{1/2}, \tag{6}$$

where β_1 is a scaling parameter equal to two.

Using the thermal balance equation for the time $\tau = \tau_1$, an approximate expression was written for the time at which surface fusion commences:

$$\tau_1 = \left[\frac{8\tau_i^4 \lambda_0 \rho c (t_f - t_0)^2}{\beta_1^2 (1 - R_0)^2 E^2}\right]^{1/3}. \tag{7}$$

Using the thermal balance equation for the time interval $\tau = \tau_2 - \tau_1$

$$(1 - R_a) E = \rho c (t_f - t_0) l, \tag{8}$$

where $l = (2\lambda_s\tau/\rho c)^{1/2}$, the duration of surface fusion was determined:

$$\tau_2 - \tau_1 = \frac{\beta_2^2 (1 - R_a)^2 E^2}{2\lambda_s \rho c (t_f - t_0)^2}, \tag{9}$$

TABLE 1. Properties of Materials [5] Used in Calculations

Parameter	Silicon	Germanium	Gallium arsenide
ρ, $g \cdot cm^{-3}$	2,33	5,32	5,31
c, $J \cdot g^{-1} K^{-1}$	0,72	0,32	0,32
λ_0, $W \cdot cm^{-1} K^{-1}$	0,51	0,28	0,18
λ_s, $W \cdot cm^{-1} K^{-1}$	0,38	0,18	0,13
t_f, K	1710	1230	1520
H, $J \cdot g^{-1}$	1970	410	620
R_0	0,35	0,40	0,30
R_a	0,50	0,60	0,50

TABLE 2. Calculated and Experimental [1, 4] Values of Minimum Energy Density in 60-nsec Laser Pulse to Produce Fusion of Specimen Surface

Material	Laser wavelength, μ	Adsorption coeff., cm^{-1}	Calculated energy density, $J \cdot cm^{-2}$	Exptl. energy density, $J \cdot cm^{-2}$
Silicon	0,53	$5 \cdot 10^4$	0,3	0,3
Silicon	0,69	$3 \cdot 10^3$	0,8	0,8
Silicon	1,06	$5 \cdot 10^2$	5,3	5,5
Germanium	0,53	$5 \cdot 10^5$	0,16	0,16
Gallium arsenide	0,53	10^5	0,12	0,10

where β_2 is a scaling parameter equal to 1.06.

As follows from numerical calculations, at $\tau \to \tau_2$ the temperature gradient in the melt is negligibly small in comparison to the temperature gradient in the unfused portion of the material, which is equal to $(t_f - t_0)/l$, where l is defined by Eq. (8). Thus, on the basis of Eq. (4) an approximate equation is obtained for the recrystallization rate of the fused layer

$$v_r = -\frac{dx}{d\tau} = \frac{\lambda_s c (t_f - t_0)^2}{\beta_3 H (1 - R_a) E}, \tag{10}$$

where β_3 is a scaling parameter equal to 1.6.

Approximating the time dependence of the position of the phase boundary by a triangle with base $\tau_2 - \tau_1$, we find the maximum fusion depth in the material:

$$L_{max} = v_r[\tau_1 + (\tau_2 - \tau_1) - \tau_L] = \frac{\lambda_s c (t_f - t_0)^2}{\beta_3 H (1 - R_a) E} \left\{ \frac{\beta_2^2 (1 - R_a)^2 E^2}{2\lambda_s \rho c (t_f - t_0)^2} + \left[\frac{8\tau_1^4 \lambda_0 \rho c (t_f - t_0)^2}{\beta_1^2 (1 - R_0)^2 E^2} \right]^{1/3} - 2\tau_1 \right\}. \tag{11}$$

On the basis of Eqs. (6)-(11) the effect on laser annealing parameters of initial specimen temperature, and pulse energy density and duration can be determined. Thus, it follows from Eqs. (9), (10) that the duration of surface fusion and the recrystallization rate are independent of laser impulse duration.

Figure 1 shows results of calculating the duration of surface fusion with Eq. (9) and experimental data from [4] for silicon, germanium, and gallium arsenide, irradiated at room temperature by a neodymium laser pulse 60 nsec long. Satisfactory agreement was also obtained for other values. Table 1 presents the properties of the materials [5] used in the calculations.

The approximate equations (6), (7), (9)-(11) describe laser annealing parameters well at $E \geqslant E_{min}$ for high absorption coefficients: $\alpha \geqslant 5 \cdot 10^4$ cm^{-1}. In the opposite case it is necessary to consider the dependence of the scale coefficients on the absorption coefficient. In the interval $5 \cdot 10^2 \leqslant \alpha \leqslant 5 \cdot 10^4$ cm^{-1} the approximate expressions produce satisfactory agreement with numerical calculation results and experimental data when the following expression is used for the scale coefficients:

$$\beta' = \beta \left\{ 1 - \exp\left[-\alpha \left(\frac{E}{E_{min}} \right)^2 \left(\frac{4\lambda_0 \tau_1}{\rho c} \right)^{1/2} \right] \right\}, \tag{12}$$

where β' is the scaling parameter for $5 \cdot 10^2 \leqslant \alpha \leqslant 5 \cdot 10^4$ cm^{-1} and β is the scaling coefficient for $\alpha \geqslant 5 \cdot 10^4$ cm^{-1}.

Equation (12) was obtained by considering the difference in the optical energies absorbed at the heat penetration depth in the specimen over the period of pulse action, and

TABLE 3. Dislocation Annealing Depth in Single-Crystal Silicon for Ruby Laser Pulses [1] and Calculated Fusion Depths

Pulse energy density, $J \cdot cm^{-2}$	Pulse half-duration, nsec	Annealing depth, μ	Fusion depth, μ
1,5	50	0,29	0,30
2,0	20	0.57	0,58
3,0	20	0,95	0,95

the fact that the temperature of the surface layer increases more rapidly with increase in laser pulse energy density, thus producing a more rapid increase in the absorption coefficient at high energies.

Table 2 presents values of minimum laser pulse energy required for fusion of silicon, germanium, and gallium arsenide surfaces for lasers radiating at various wavelengths. The calculated values are compared with experimental data from [1, 4].

Table 3 presents parameters for dislocation annealing in single-crystal silicon by ruby laser pulses as well as fusion depths calculated with Eq. (11).

As follows from comparison of the experimental data with results of calculations using Eqs. (6), (7), (9)-(12), use of the approximate expressions makes it possible to select technological regimes for processing semiconductor materials, in particular, for annealing defects, producing p–n junctions, and ohmic contacts.

NOTATION

d, diameter of irradiated region; λ, thermal conductivity; τ, time; ρ, density; c, specific heat; t, temperature; x, depth (distance from specimen surface); $q(x, \tau)$, heat source; α, absorption coefficient; R, reflection coefficient; $I(\tau)$, power density of incident laser impulse; τ_i, one half of pulse duration; I_{max}, maximum power density of incident laser impulse; t_0, initial temperature; λ_s, thermal conductivity of material in the solid state at fusion; λ_l, thermal conductivity of material in the liquid state at fusion temperature; H, latent heat of fusion; τ_1, time at which fusion of specimen surface begins; L_{max}, maximum fusion depth; t_{max}, maximum surface temperature; τ_L, time required for fusion of specimen to maximum depth; τ_t, time required to achieve maximum surface temperature; t_f, fusion point of speciment material; R_0, reflection coefficient of specimen material in solid state; λ_0, specimen thermal conductivity averaged over temperature range from t_0 to t_f; β_1, β_2, and β_3, scaling coefficients; l, effective depth to which heat penetrates specimen; τ_2, time at which fusion of specimen surface is completed; R_a, reflection material of coefficient averaged between solid and liquid states.

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