CALCULATION OF TEMPERATURE FIELDS IN A SILICON FILM DURING AN OPTICAL ANNEAL

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We consider a theoretical method for the calculation of temperature fields in silicon films during a pulsed optical anneal.

In recent years, together with works on laser annealing, papers have appeared which were devoted to the pulsed optical annealing of radiation defects and impurity activation in ion-implanted layers of semiconductor films, in the process of formation of active elements [1-4]. Having the same merits as the laser anneal, the pulsed optical anneal has a number of advantages: a relative simplicity of the method, sufficiently high reproducibility of the process, no redistribution of the implanted impurity during the anneal, absence of negative side effects, etc.

To discuss the regimes of the pulsed optical anneal, it is necessary to know with a sufficient accuracy the temperature on the surface of the silicon film, and the temperature profile along its thickness. Since there are no devices at present which can measure temperature of small objects during the time of the order of 10 msec, it is impossible to obtain this information experimentally. Calculation using the simplified formulas [5] is difficult and lacks sufficient accuracy. We have therefore found it necessary to determine the temperature at the surface of the film and the temperature profile with respect to its thickness by a calculation.

For the silicon films under consideration (which were of thickness $\delta \sim 350\ \mu\mathrm{m}$ with the absorption coefficient $k \sim 10^4\ \mathrm{cm}^{-1}$ [5]) one can use the assumption of optically infinitely thick plane layer, since the absorption of radiation takes place in the thickness of several microns. In this case, the layer which is transparent to the radiation contains predominantly the direct light flux, and the secondary scattering effects can be neglected due to their low orders [6]. The problem of finding the temperature fields during light irradiation of semiconducting films is then described by a nonlinear differential equation of the same type as the heat-conduction equation, with an internal heat source which is due to the absorption of infrared radiation in the layer.

In dimensionless coordinates, the equation can be written as

$$\frac{\partial\Theta(\xi,\ \mathrm{Fo})}{\partial \mathrm{Fo}} = \frac{\partial^2\Theta(\xi,\ \mathrm{Fo})}{\partial\xi^2} + \mathrm{Ki}\,\mathrm{Bu}\exp(-\mathrm{Bu}\,\xi) \tag{1}$$

with the initial condition

$$\Theta(\xi,\ 0) = \Theta_0(\xi) \tag{2}$$

and the boundary conditions

$$\frac{\partial\Theta(0,\ \mathrm{Fo})}{\partial\xi} = \mathrm{Bi}\,[\Theta(0,\ \mathrm{Fo}) - 1], \tag{3}$$

$$-\frac{\partial\Theta(1,\ \mathrm{Fo})}{\partial\xi} = \mathrm{Bi}\,[\Theta(1,\ \mathrm{Fo}) - 1]. \tag{4}$$

Here we assumed that the light pulse has a rectangular temporal form and the spatial distribution of the incident radiation is uniform.

In general, the coefficients a_m, λ, α_m, k in the dimensionless criterium are variable quantities but, for simplicity of calculation, we use constant values of the coefficients taken from [1, 7].

The solution of the problem (1)-(4) will be sought in the rectangle $\Pi = \{0 \leqslant \xi \leqslant 1;\ 0 \leqslant \mathrm{Fo} \leqslant \mathrm{Fo}^*\}$ by the mesh method [8]. In Π we consider the mesh of nodes $\omega_{h\tau} = \{\xi_i = ih,\ h > 0,\ i = 0,\ 1,\ \ldots,\ N;\ Nh = 1;\ \mathrm{Fo}_j = j\tau,\ \tau > 0,\ j = 0,\ 1,\ \ldots,\ M;\ M\tau = \mathrm{Fo}^*\}$, and on this mesh we construct the following implicit difference scheme:

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$$y_t = \hat{y}_{\bar{x}x} + \mathrm{Ki\,Bu}\exp(-\mathrm{Bu}\,\xi), \tag{5}$$

$$y(\xi_i,\ 0) = y_{i0}, \quad i = 0,\ 1,\ \ldots,\ N, \tag{6}$$

$$\hat{y}_{x,0} = \mathrm{Bi}\,(\hat{y}_0 - 1), \quad \hat{y}_{\bar{x},N} = -\mathrm{Bi}\,(\hat{y}_N - 1), \tag{7}$$

where $y = y_{ij} = \Theta_{ij}$ is the approximate value of Θ in point $\xi = \xi_i$, $\mathrm{Fo} = \mathrm{Fo}_j$; $\hat{y} = y_{ij+1}$; $y_t = (\hat{y} - y)/\tau$; $\hat{y}_x = (y_{i+1,j+1} - y_{i,j+1})/h$; $\hat{y}_{\bar{x}} = (y_{i,j+1} - y_{i-1,j+1})/h$; $\hat{y}_{\bar{x}x} = (\hat{y}_x - y_{\bar{x}})/h$. The difference scheme (5)-(7) approximates the original problem (1)-(4) with error $O(\tau + h)$ and is absolutely stable. In addition, the rate of convergence of this algorithm coincides with the order of the error of the approximation.

Let us suppose that for $\mathrm{Fo} = \mathrm{Fo}_j$, the solution has been determined. To find the solution for $\mathrm{Fo} = \mathrm{Fo}_{j+1}$, we then obtain from (5)-(7) a system of N + 1 linear algebraic equations

$$\begin{gathered} \frac{\tau}{h^2}\,\hat{y}_{i-1} - \left(\frac{2\tau}{h^2} + 1\right)\hat{y}_i + \frac{\tau}{h^2}\,\hat{y}_{i+1} = -[y_i + \tau\,\mathrm{Ki\,Bu}\exp(-\mathrm{Bu}\,\xi_i)], \quad i = 1,\ 2,\ \ldots,\ N-1, \\ \hat{y}_1 - \hat{y}_0 = h\,\mathrm{Bi}\,(\hat{y}_0 - 1), \quad \hat{y}_N - \hat{y}_{N-1} = -h\,\mathrm{Bi}\,(\hat{y}_N - 1) \end{gathered} \tag{8}$$

with respect to N + 1 unknowns $\hat{y}_0,\ \hat{y}_1,\ \ldots,\ \hat{y}_N$. For the realization of the difference scheme (8), we shall use a three-point difference driving method. To this end, we introduce the following notation: $a = \tau/h^2$, $c = 2\tau/h^2 + 1$, $F_j = y_j + \tau\,\mathrm{Ki\,Bu}\exp(-\mathrm{Bu}\,\xi_i)$, $\varkappa = (1 + h\,\mathrm{Bi})^{-1}$, $\nu = h\,\mathrm{Bi}\,\varkappa$. The system (8) is then transformed to

$$\begin{gathered} a\hat{y}_{i-1} - c\hat{y}_i + a\hat{y}_{i+1} = -F_i, \quad i = 1,\ 2,\ \ldots,\ N-1; \\ \hat{y}_0 = \varkappa\,\hat{y}_1 + \nu, \quad \hat{y}_N = \varkappa\hat{y}_{N-1} + \nu. \end{gathered} \tag{9}$$

The solution of (9) will be sought in the form

$$\hat{y}_i = \alpha_{i+1}\hat{y}_{i+1} + \beta_{i+1}, \quad i = 0,\ 1,\ \ldots,\ N-1, \tag{10}$$

where, following the difference driving method, α_{i+1} and β_{i+1} are determined from the relations $\alpha_{i+1} = a/(c - a\alpha_i)$, $\beta_{i+1} = (a\beta_i + F_i)/(c_i - a\alpha_i)$, $i = 1,\ 2,\ \ldots,\ N-1$, $\alpha_1 - \varkappa$, $\beta_1 = \nu$, , and $\hat{y}_N$ is obtained by using the second boundary condition: $\hat{y}_N = (\nu + \varkappa\beta_N)/(1 - \varkappa\alpha_N)$.

Knowing α_{i+1}, β_{i+1} and y_N, all $\hat{y}_i$($i = N - 1, N - 2, \ldots, 1, 0$) can be determined recurrently from relation (10). For $\mathrm{Bi} > 0$, the algorithms of the driving method is stable.

Control calculations of the problem (1)-(4) using the difference scheme (5)-(7) were carried out for $h = 10^{-3}$ (step τ can be arbitrary). The computation time t_c then obeys the law $t_c = bM$ (min), where b = 0.04 for the Minsk-32 computer. For example, the computation time of the problem in II for Fo = 8.8, and $\tau = 0.1$ was 3.52 min.

We note that the problem of optical annealing of films in the present formulation allows an analytical solution [9]. However, to obtain the numerical value of the solution from the analytic form is more complicated since the program for the realization of the algorithm becomes more complicated. The algorithm presented here is universal and can be used for the solution of more complicated problems with other heat sources and nonlinear boundary conditions.

The calculation of the temperature profiles with respect to the depth of the silicon film during its illumination by light pulses was carried out using parameters given in Table 1.

Figure 1 shows the calculated temperature profiles for two energy values. It is seen that when the duration of the light pulse is decreased from 14 to 8 msec with W = 80 J/cm^2, the temperature on the surface of the sample increases from 1224 to 1605°C, and the temperature drop across the thickness of the sample also increases, from 96 to 167°C. For W = 100 J/cm^2, the temperature on the surface of the film increases from 1470 to 1954°C when the pulse duration is decreased. The temperature drop here increases from 123 to 217°C.

The agreement of the presented mathematical model and the real annealing process in silicon films was tested experimentally by observing the beginning of melting of silicon on the illuminated side (T_m = 1412°C), and the melting of copper films (T_m = 1083°C) and aluminum films (T_m = 658°C) on the reverse side. The thickness of the copper and aluminum films was 0.5-1 μm, and one can therefore neglect the effect of the film on the temperature field in the silicon film. In the

TABLE 1. Parameters of the Energetic Interaction during a Pulsed Anneal of Silicon Films

W, J/cm^2	60	80				100				120		
$t^* \cdot 10^3$, sec	14	8	10	12	14	8	10	12	14	8	10	12
$q_f \cdot 10^{-3}$, W/cm^2	4,3	10	8	6,65	5,7	12,5	10	8,35	7,15	15	12	10

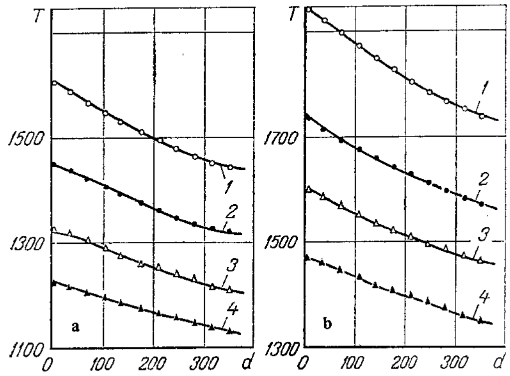

Fig. 1. Comparison of the temperature profiles with respect to the thickness of the silicon film for various durations of the light pulses with energy W = 80 J/cm^2 (a) and W = 100 J/cm^2(b). 1) t* = 8; 2) 10; 3) 12; 4) 14 msec. The temperature T is in °C and d is in μm.

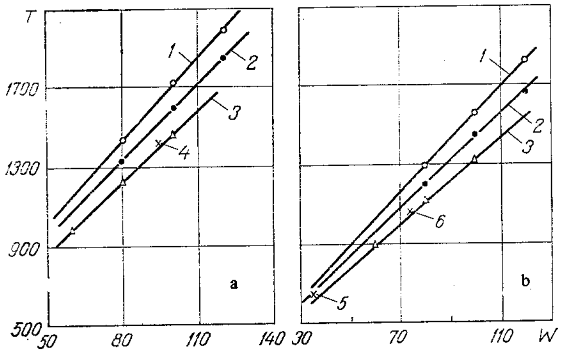

Fig. 2. Comparison of theoretical values of the temperature on the illuminated (a) and reverse (b) surfaces of the silicon film. 1) t* = 10; 2) 12; 3) 14 msec; 4) temperature of melting silicon; 5, 6) temperature of melting aluminum and copper, respectively.

experiment, we used silicon films of diameter 60 mm and thickness $\delta \approx 350$ μm. The anneal was done by three pulsed lamps of type IFP-8000 with pulse duration 8-14 msec. The energy of the light pulse depended on the annealing impurity, dose, and the implanting energy and was specified by charging condenser batteries up to appropriate voltage (in the limits 2.2-4.1 kV).

Figure 2 shows the theoretical dependence of the temperature on the illuminated and reverse sides of the silicon film, on the incident energy density. Shown are the obtained experimental points which characterize the beginning of melting of the differential materials. It was established in the experiment that, for a light pulse of duration 14 msec, silicon begins to melt at incident energy W = 94, copper at 74, and aluminum at 35 J/cm^2. Figure 2 shows a good agreement of the experimental and theoretical data.

Thus, the developed method for the calculation of temperature fields in semiconducting films can be used to analyze the regimes of pulsed optical anneal of ion-implanted layers.

NOTATION

a_m, thermal diffusivity; A, silicon absorptivity; k, α_m, and λ, absorption, heat exchange, and thermal conductivity coefficients; δ, thickness of the silicon film; q_f, heat flux density; t*, duration of the light pulse; W, pulse energy; $\Theta = T(x, t)/T_0$, dimensionless temperature; $\xi = x/\delta$, dimensionless coordinate; h and τ, space and time steps; $Bi = \alpha_m \delta/\lambda$, Biot number; $Ki = Aq_d\delta/\lambda\ T_0$, Kirpichev number; $Bu = k\delta$, Bouger number; and $Fo = a_m t/\delta^2$, Fourier number.

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NUMERICAL METHOD FOR SOLVING THE COUPLED PROBLEM OF RADIATIVE–CONVECTIVE AND CONDUCTIVE HEAT TRANSFER

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The solution of the problem of complex heat transfer is reduced to a systematic solution of a system of nonlinear equations and the heat-conduction equations. A rapid iterative method is proposed for solving the system of equations.

The problem of heating and cooling of a system of bodies with a complex shape under conditions of radiation–convection heat transfer has not been adequately studied. The case when the bodies are heated in a regular regime was examined in [1]. For nonstationary processes, this assumption is not satisfied.

We shall examine a radiating volume V, surrounded by a system of opaque bodies. The surface F of the volume V consists of the surfaces of the bodies and of "liquid" boundaries, through which the heat carrier enters and leaves the volume. We shall view the latter as fictitious surfaces, allowing gas to pass freely through them. These surfaces are assigned a certain temperature (or flux density of the resulting radiation), as well as an effective emissivity. This artificial technique is used quite frequently [2] to close the emitting system in examining radiative transfer and permits the gas flow to leave the system at the same time.

We shall divide the volume V and the bounding surface F into N zones. For each zone n, we shall write the law of conservation of energy in the form

$$Q_{\text{rad.},n} = -Q_n,\ n = 1,\ 2,\ \ldots,\ N. \tag{1}$$

The radiant energy transport is approximated using the resolvent method by a system of algebraic equations

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