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INFLUENCE OF THE INITIAL TEMPERATURE OF SILICON ON CRYSTALLIZATION OF A LAYER MELTED BY NANOSECOND LASER HEATING

S. P. Zhvavyi and G. D. Ivlev

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The effect of the initial temperature of silicon on the dynamics of phase transitions induced by nanosecond laser heating was studied on the basis of numerical solution of the Stefan problem.

The basic parameter determining impurity behavior and the change in the structural state of silicon in nanosecond heating by laser radiation is the rate of crystallization of the melt v_c [1], which depends on the pulse duration, energy density, and the coefficient of radiation absorption in the semiconductor, which at the initial stage of crystallization amounts to 1 – 10 m/sec. By changing the initial temperature of the substrate one can effectively control the value of v_c [2, 3] and thus substantially decelerate the crystallization process and prolong the time of melt existence. The latter fact, for instance, allows one to considerably increase the size of single-crystal regions of silicon on a dielectric interlayer that are formed by lateral crystallization of a melted layer with a seed from the basic monocrystal [4]. Phase transitions which occur in silicon under the effect of nanosecond laser pulses under conditions of additional heating of the substrate have not, however, been studied as yet in real time, except in [5]. In [5], by the method of optical probing, the dynamics of recrystallization of a polysilicon film separated from a monocrystal substrate by a dielectric layer was studied. A certain idea about the specific features of the dynamics of the mentioned phase transitions is given only by the results of numerical simulation conducted, in particular, in [2, 3].

In this paper the dynamics of phase transitions occurring in monocrystal silicon under the effect of nanosecond pulses of a ruby laser with variation of the sample initial temperature within a wide range was studied experimentally. The data obtained are compared with the results of numerical solution of the heat conduction equation.

Laser irradiation of KDB-20 silicon wafers with orientation (100) was conducted under the experimental conditions of [5] with a pulse duration of 70 nsec and a spot diameter of 3–5 mm. The sample was placed in a chamber with halogen lamps, where it was heated to a certain temperature controlled by a thermocouple. The dynamics of reflection of the probing radiation focused on the center of the irradiated region was registered by an FEU ELU-FTK photomultiplier and an S8-14 oscillograph. The time of melt existence at various initial temperatures of the sample, whose maximum value was 1000 K, was found from the oscillograms.

The numerical simulation of melting and crystallization of silicon was conducted by the method of finite differences. A one-dimensional approximation was used in accordance with which the change in the silicon temperature under the effect of a nanosecond laser pulse is described by the heat conduction equation

$$\rho (T) [c (T) + L_m \delta (T - T_m)] \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left[k (T) \frac{\partial T}{\partial x} \right] + S (x, t) \tag{1}$$

and by the boundary and initial conditions

$$\left. \frac{\partial T}{\partial x} \right|_{x=0} = 0 , \quad T (x \to \infty, t) = T_0 , \quad T (x, t = 0) = T_0 ,$$

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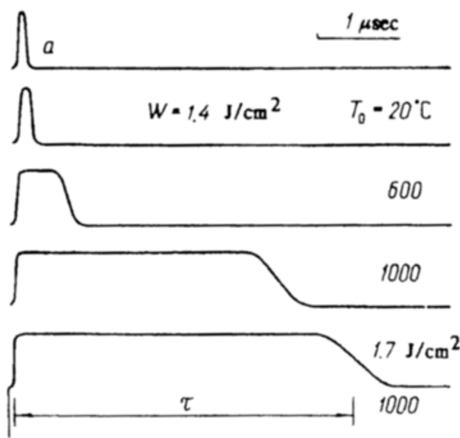

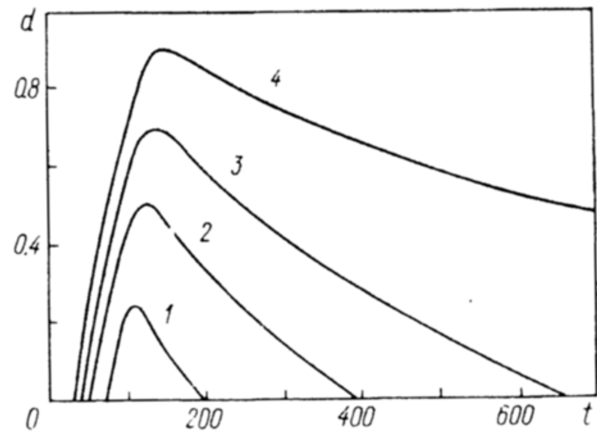

Fig. 1. Oscillograms of laser pulse (a) and probing-radiation reflection from silicon. τ, time of liquid-phase existence.

Fig. 2. Time dependences of the thickness of the melted silicon layer at $W = 1.4$ J/cm^2 and different values of the initial temperature T_0: 1) 20 °C; 2) 400; 3) 700; 4) 1000. d, μm; t, nsec.

where ρ is the density, c is the specific heat capacity, k is the coefficient of thermal conductivity, L_m is the latent heat of melting, T_m is the melting temperature, T_0 is the initial temperature, $\delta(x)$ is the δ-function. The heat source $S(x, t)$ in (1) describes heat release due to laser radiation absorption:

$$S(x, t) = (1 - R)\, \alpha(x, T) \frac{W(t)}{\tau_p} \exp\left[-\int_0^x \alpha(x', T)\, dx'\right],$$

where R and α are the coefficients of reflection and absorption, W and τ_p are the energy density and laser pulse duration.

The introduction of the term with the δ-function on the left-hand side of Eq. (1) allowed one to solve numerically the heat conduction equation by the method of through calculation without explicit selection of a phase interface. In composing an implicit difference scheme the method of smoothing was used [6], according to which the δ-function was approximated by a δ-like function of the form

$$\delta(T - T_m, \Delta) = \frac{1}{\sqrt{2\pi}\,\Delta} \exp\left[-\frac{(T - T_m)^2}{2\Delta^2}\right]$$

with the initial width $\Delta = 10$ °C, which, depending on the temperature gradient, varied such that the range of definition of the δ-like function covered not less than three calculation points. At the phase interface the smoothed effective coefficient of heat conduction was also introduced. The problem was solved by the pivot method using an iteration process. The spatial step was variable from $h = 0.01$ μm for $0 < x \le 1$ μm to $h = 0.5$ μm for $20 < x < 35$ μm, since the temperature gradient near the surface substantially exceeds that in the depth of the irradiated sample. The initial time step was 0.2 nsec and could change depending on the convergence of iterations during calculations. The shape of the laser pulse was assigned by the function $\sin^2(\pi t/2\tau_p)$, where $\tau_p = 70$ nsec. The velocity of motion of the liquid–solid phase interface was found from the condition

$$L_m \rho v = k_s \left(\frac{\partial T}{\partial x}\right)_s - k_{liq} \left(\frac{\partial T}{\partial x}\right)_{liq}.$$

The values of the thermophysical and optical parameters used in the calculations are given in the Table 1. In accordance with the data (Fig. 1) an increase in T_0 to 1000 K leads to a considerable (by more than an order) increase in the time of the existence of a melted layer. Here the calculated depth of melt penetration (Fig. 2) grows

TABLE 1. Physical Properties of Silicon

Parameters	Crystalline	Melted
ρ, g/cm^3	2.328	$2.53-0.152\cdot10^{-3}(T-T_m)$ [7]
c, J/(g·K)	$0.844+1.18\cdot10^{-4}T-1.55\cdot10^{4}T^{-2}$ [7]	0.97
L_m, J/g	1787 [7]	
k, W/(cm·K)	$1521/T^{1.226}$ when $T\le1200$ K; $8.97/T^{1/2}$ when $T>1200$ K [8]	0.585 [7]
α, cm^{-1}	1578 exp $(T/493)$ [9]	10^6
R	0.32	0.72

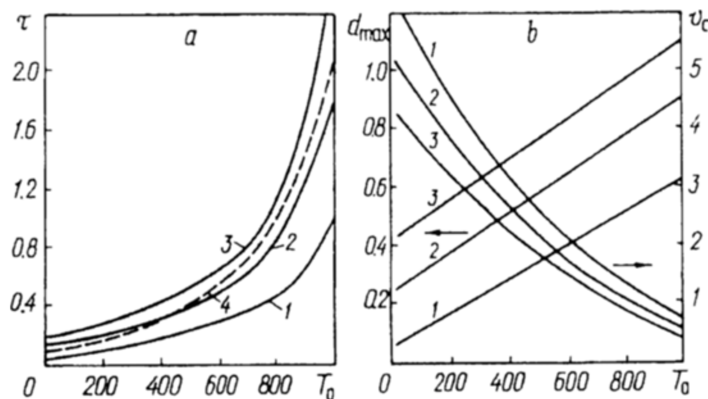

Fig. 3. Dependences of the time of melt existence (a), maximum depth of melting d_{max}, and final rate of crystallization v_c (b) on the initial temperature at different values of W, J/cm^2: 1) 1; 2) 1.4; 3) 1.7. Dashed curve – experimental dependence of τ. τ, μsec; d_{max}, μm; v_c, m/sec; T, °C.

by about 4 times, approaching 1 μm. A comparison of the experimental values of $\tau(W)$ with the calculational ones (Fig. 3a) shows that they differ by not more than 15–20%. In the range of temperatures of from 20 to 600 K the dependence $\tau(T_0)$ is close to linear. When $T_0 > 600$ K, a sharp increase in τ with T_0 is observed that is caused by a considerable decrease in the velocity of motion of the phase-interface front. The latter is explained by substantial deterioration of the conditions of heat removal from the phase interface, on which latent heat of phase transition is liberated, due to a decrease in the temperature gradient and the coefficient of heat conduction $k \sim T^{-1/2}$, since at this time the temperature of the main region is much lower than the melting point. As the phase interface reaches the surface, the rate of crystallization changes within the studied range of T_0 variation by about as many times as the value of τ (Fig. 3b). It is noteworthy that the depth of melting grows proportionally to T_0, with the coefficient of proportionality being practically the same for three values of the energy density of laser radiation and amounting to $\sim 6\cdot10^{-4}$ μm/K. It should be also mentioned that the maximum calculated temperature of the melt surface within the studied range of T_0 variation changes not as much as would be expected. For example, it grows from 1725 K (T_0 = 20 K) to 2070 K (1000 K) at W = 1.7 J/cm^2. At an energy density of 1.4 J/cm^2, it increases only by 350 K, amounting to 1565 K without additional heating.

The study conducted shows that experimental data on the dynamics of phase transitions in silicon that occur under the effect of nanosecond laser radiation with varying initial temperature of the solid phase are in satisfactory agreement with the results of solution of the equation of heat conduction in a diffuse approximation. It is found that a nonlinear increase in the period of liquid-phase existence, depending on the initial temperature of silicon, is caused by substantial retardation of the crystallization process. The depth of silicon melting is linearly

dependent on the initial temperature, i.e., on the specific heat energy accumulated in the semiconductor as a result of additional heating.

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