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BRIEF COMMUNICATIONS

Diffusion of As Ions and Self-Diffusion in Silicon During Implantation

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Abstract—Experimental concentration profiles of As ions in a silicon substrate at the temperatures of 20, 600, and 1050°C and the ion current of 40 μA/cm^2, as well as at 1050°C and 10 μA/cm^2, are presented. On the basis of our and previously published experimental data, the process of radiation-stimulated ionic diffusion and self-diffusion in silicon is simulated. A number of interesting dependences, discussed in the conclusion of this study, are obtained. *© 2002 MAIK "Nauka/Interperiodica".*

INTRODUCTION

The investigation of the behavior of different impurity ions implanted into semiconductor materials as functions of current density, ambient temperature, exposure time, ion energy, and the chemical properties of interacting substances is of great theoretical and practical importance. In this study, we investigate the implantation of 40-keV As ions into a silicon substrate in a wide temperature range.

EXPERIMENTAL

In our experiments, silicon substrates were irradiated using an ILU-3 accelerator [1]. For heating the substrates in the course of irradiation, a special high-temperature ion collector was developed. As a substrate material, we used single-crystalline silicon. The implantation was performed with 40-keV As ions at a dose of 2×10^{17} ion/cm^2. The distribution of implanted atoms with depth was analyzed using X-ray diffraction with layer-by-layer etching. The main irradiation parameters are listed in Table 1. The measured concentration profiles are shown in Figs. 1 and 2. It can be seen that, even for room-temperature irradiation, the profile contains a deep-lying maximum.

THEORY

In order to explain the impurity drift into the bulk, which strongly exceeds the ion range, we applied the modified Beloshitskiĭ model [2] described previously in [3]. In addition to diffusion transport, it is assumed that impurity capture by vacancies also takes place. Note that the purely diffusion equation in the presence of a source does not have a solution with a maximum located at a greater distance from the surface than the ion range. The key feature of the model consists in its nonequilibrium—diffusion occurs against a background of intense production and annihilation of defects. These processes are described by the following

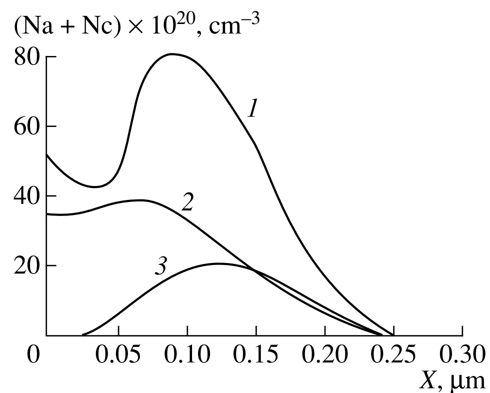

Fig. 1. Experimental concentration profiles of As in silicon at the temperatures of (*1*) 20, (*2*) 600, and (*3*) 1050°C (40 μA/cm^2).

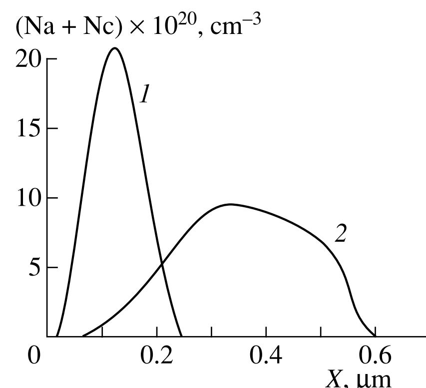

Fig. 2. Experimental concentration profiles of As in silicon for the currents (*1*) 40 and (*2*) 10 μA/cm^2 (1050°C).

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Table 1. Basic experimental parameters of the implantation of As ions with an energy of 40 keV and a dose as high as 2×10^{17} ion/cm^2

Number	T, °C	j_0, $\frac{\mu A}{cm^2}$	$\mathcal{D}_{exp}$, $\frac{ion}{cm^2} \times 10^6$	$V_{b\,exp}$, $\frac{cm}{s} \times 10^{-10}$	t_{max}, s
1	1050	10	3.101	1.940	3200
2	1050	40	2.472	6.184	800
3	600	40	11.210	28.048	800
4	20	40	5.661	14.164	800

Table 2. Calculated diffusion coefficients and enthalpies

Number	D_a, $\frac{cm^2}{s} \times 10^{-11}$	D_{dv}, $\frac{cm^2}{s} \times 10^{-11}$	H_{dv}, cal/mol	T_{eff}, °K
1	0.169	0.204	64610	1326
2	0.540	0.0633	68151	1335
3	0.007	0.0463	47157	913
4	0.499	0.0127	31937	589

system of coupled equations:

$$\partial n_a/\partial t = D_a \partial^2 n_a/\partial x^2 - n_a n_v k_{cap} + n_c n_d k_{act} + j_0 \exp(-(R_p - x + x_0)^2/2\Delta R_p^2)/\sqrt{2\pi}\Delta R_p, \quad (1)$$

$$\partial n_c/\partial t = n_a n_v k_{cap} - n_c n_d k_{act}, \quad (2)$$

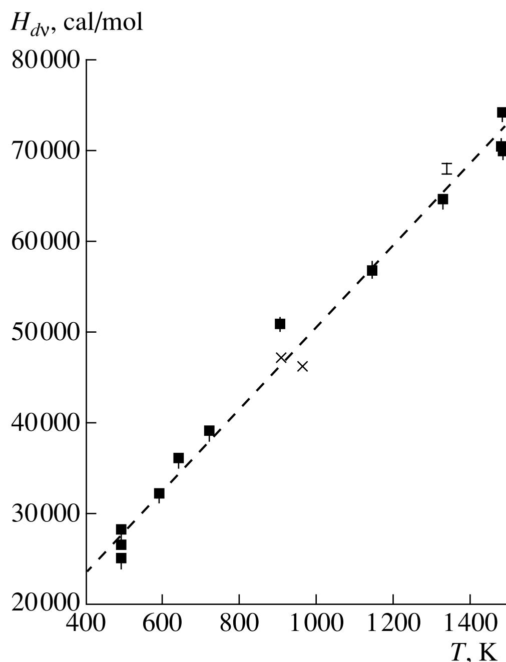

Fig. 3. Temperature dependence of the enthalpy of defect migration in silicon on the basis of the data from Tables 2 and 4.

$$\partial n_d/\partial t = D_{dv} \partial^2 n_d/\partial x^2 - n_c n_d k_{act} - n_v n_d k_{ann} + j_0 N \sigma_d \Theta(R_p - x + x_0), \quad (3)$$

$$\partial n_v/\partial t = D_{dv} \partial^2 n_v/\partial x^2 - n_a n_v k_{cap} - n_v n_d k_{ann} + j_0 N \sigma_d \Theta(R_p - x + x_0),$$
$$X_0 = -v_b t, \quad N = 5.04 \times 10^{22} \text{ cm}^{-3},$$
$$\sigma_d = 3.52 \times 10^{-16} \text{ cm}^2, \quad (4)$$

Here, $\Theta(x)$ is the unit step; N is the density of the silicon nuclei; σ_d is the approximate cross section of the defect formation; R_p and ΔR_p are the ion range and its standard deviation, respectively; and D_a, D_{dv}, k_{cap}, k_{act}, and k_{ann} are the free parameters of the model, which have the evident physical meaning of the impurity diffusion coefficient, the diffusion coefficient of the defect–vacancy pairs, the rate of the quasi-chemical reactions responsible for the impurity capture by the vacancies, the activation rate of the impurities by the interstitial atoms, and the rate of the mutual annihilation of the vacancies and interstitial atoms, respectively.

Based on the experimental data, the boundary condition for the impurity was taken to be equal to zero, which can be interpreted as its escape to the sample surface. For the interstitial atoms and vacancies such a condition was used, so that the flux of the interstitial atoms would lead to the motion of the material boundary with a velocity of v_b (the problem of Stefan type). The initial conditions and the boundary conditions at the other boundary were taken also to be equal to zero. Under the above conditions, the system of Eqs. (1–4)

Table 3. Calculated rates of the quasi-chemical reactions

Number	K_{cap}, $\frac{cm^2}{s} \times 10^{-23}$	K_{act}, $\frac{cm^2}{s} \times 10^{-23}$	K_{ann}, $\frac{cm^2}{s} \times 10^{-23}$
1	2.355	7.421	2.609
2	0.889	8.321	5.795
3	0.943	15.60	5.763
4	0.929	8.260	5.855

Table 4. Calculated enthalpies for the other experiments

Ion	T, °C	j_0, $\frac{\mu A}{cm^2}$	E, keV	T_{eff}, K	H_{dv}, $\frac{cal}{mol}$	Reference
Yb	20	10	70	488	27811*	[5, 6]
					26877	
					24697	
Na	365	0.3	7	638	35845	[7]
As	20	150	25	722	38703	[8]
Tm	500	30	150	906	50900	[9]
C	20	300	40	961	46377*	[2, 10]
					46931	
					47058	
As	850	40	40	1143	57164	[12]
Tl	1200	40	20	1478	70591	[3]
As	1200	40	40	1482	74154	[11]
Tl	1200	100	20	1484	70064	[4]

* For pure silicon (further, growth in the impurity concentration).

was solved numerically using a computer and the finite-difference scheme. The values of the free parameters in our model were fitted by the least-squares method in such a way that they corresponded as close as possible to the experimental profiles.

CONCLUSION

The results of the calculations are listed in Tables 2 and 3. In Table 2, in addition, the enthalpies of defect migrations (evaluated by the Arrhenius equation) and the effective temperatures of the surface layer (with allowance made for the beam-induced heating) are also presented. In Table 4, the data from our additional calculations of the enthalpy of silicon self-diffusion are listed. Figure 3 shows the temperature dependence of the enthalpy of the defect migration, which was obtained using the data from Tables 3 and 4.

As can be seen from Fig. 2, in contrast to our results obtained for the implantation of Tl ions into silicon [3, 4], the profile strongly depends on the As ion current.

From Table 4, one can see the dose dependences of the enthalpy of defect migrations for the impurity ions of carbon and ytterbium in silicon, which are of opposite character. Note that the ytterbium ions migrate to the surface, whereas the carbon ions migrate into the bulk of a sample.

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