

BRIEF COMMUNICATIONS

## Anomalous Behavior of Arsenic Ions Implanted into Silicon at 850°C

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**Abstract**—The concentration profile of arsenic in silicon was found to have two peaks at large depths. An implantation model is suggested. A comparison with results for other species is made. It is shown that mechanisms behind low- and high-temperature migrations of defect–vacancy pairs are similar to each other ( $D_{dv}$  is about  $10^{-12}$  cm<sup>2</sup>/s). © 2001 MAIK “Nauka/Interperiodica”.

### INTRODUCTION

The behavior of implanted ions in semiconductor materials according to ion current density and ion energy, temperature of the material, and chemical properties of interacting substances is of great theoretical and applied importance. In this work, we studied arsenic implantation (40 keV, 40 μA/cm<sup>2</sup>) into a silicon target at a high temperature (850°C).

### EXPERIMENT

Irradiation was carried out in an ILU-3 ion-beam accelerator [3]. During irradiation, the target (single-crystal silicon) was heated with a special high-temperature ion collector. The implantation dose was  $2 \times 10^{17}$  ion/cm<sup>2</sup>. The ion distribution in the target was studied by X-ray diffraction analysis combined with layer-by-layer etching. The profile measured is depicted in the figure. It differs from the conventional profiles by the presence of two “deep-seating” maxima.

### THEORETICAL MODEL

To explain impurity drift to a depth that is much greater than the ion range at implantation, we invoked the modified Beloshitsky model [2, 3]. In this model, it is assumed that diffusion transfer is accompanied by impurity capture by vacancies. Note that, in the presence of a source, the purely diffusion equation does not yield a peak beyond the ion range. Importantly, the model is nonequilibrium: diffusion proceeds in parallel with defect generation and annihilation. These processes are described by the set of coupled equations

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

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

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

$$\begin{aligned} \partial n_v / \partial t = D_{dv} \partial^2 n_v / \partial x^2 - n_a n_v k_{cap} - n_v n_d k_{ann} \\ + j_0 N \sigma_d \Theta(R_p - x + x_0), \end{aligned}$$

$$\begin{aligned} x_0 = -v_b t, \quad N = 5.04 \times 10^{22} \text{ cm}^{-3}, \\ \sigma_d = 3.52 \times 10^{-16} \text{ cm}^2, \end{aligned} \quad (4)$$

Here,  $\Theta(x)$  is a unit step;  $N$  is the density of silicon

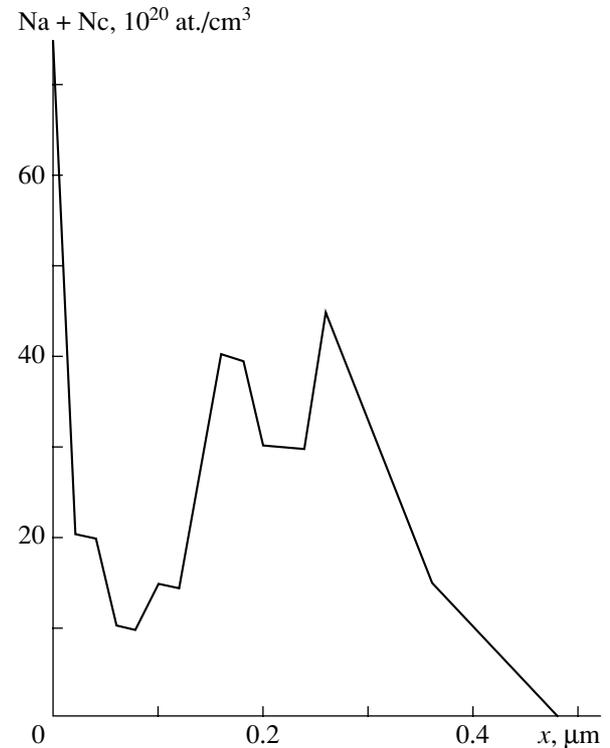


Figure.

Table 1

$D_a, \frac{\text{cm}^2}{\text{s}} \times 10^{-11}$	$D_{dv}, \frac{\text{cm}^2}{\text{s}} \times 10^{-11}$
0.199	0.1070
53.630	0.1037

nuclei;  $\sigma_d$  is the tentative cross section of defect formation;  $R_p$  and  $\Delta R_p$  is the projected ion range and its scatter, respectively; and  $D_a$ ,  $D_{dv}$ ,  $k_{cap}$ ,  $k_{act}$ , and  $k_{ann}$  are free model parameters that have the obvious meaning of diffusion coefficients of impurity and defects and rate constants for impurity capture by vacancies, impurity activation by interstitials, and vacancy–interstitial annihilation.

The boundary condition for the impurity concentration was set equal to zero; in other words, the impurity was believed to evaporate from the surface, following the experimental observation. It was assumed that the flux of interstitials causes the material boundary to shift with a rate  $v_b$  (Stefan-type problem). For interstitials and vacancies, the initial conditions and those at the opposite boundary were also zero. It should be noted that, within our model, an experimental profile can be described by only two sets of the free parameters. System (1)–(4) with the above initial and boundary conditions was numerically solved by the finite difference method. The free parameters were adjusted by the least squares technique so as to provide the best fit to experimental profiles. The associated data are summarized in Tables 1 and 2.

## CONCLUSION

### *Comparison with Results for Other Species*

In [4], concentration profiles of molecular and atomic hydrogen implanted (600 eV,  $2.5 \mu\text{A}/\text{cm}^2$ ) at 40 K were studied using the  $^1\text{H}(^{15}\text{N}, \alpha\gamma)^{15}\text{C}$  resonance reaction. We obtained similar diffusion coefficients for Frenkel pairs ( $0.107 \times 10^{-11} \text{ cm}^2/\text{s}$ ). Noteworthy, however, is the much higher quasi-chemical activity of molecular hydrogen (compared with atomic hydrogen)

Table 2

$k_{cap}, \frac{\text{cm}^2}{\text{s}} \times 10^{-23}$	$k_{act}, \frac{\text{cm}^2}{\text{s}} \times 10^{-23}$	$k_{ann}, \frac{\text{cm}^2}{\text{s}} \times 10^{-23}$
3.005	13.315	3.852
19.582	6.743	1.872

in reactions of impurity capture, Frenkel pair annihilation, and impurity activation (by a factor of 76.21, 83387.1, and 12.194, respectively). We also determined the diffusion coefficients for molecular and free hydrogen in Si ( $2.522 \times 10^{-11}$  and  $1.512 \times 10^{-11} \text{ cm}^2/\text{s}$ , respectively). The low- and high-temperature diffusion coefficients for Frenkel pairs in Si nearly coincide (Tables 1, 2). These values are close to  $0.101 \times 10^{-11} \text{ cm}^2/\text{s}$ , which was obtained by us from data [5] for deuterium implantation (27 keV,  $400 \mu\text{A}/\text{cm}^2$ ) into diamond-like carbon films at room temperature. The diffusion coefficients of deuterium in C ( $2.612 \times 10^{-11} \text{ cm}^2/\text{s}$ ) and molecular hydrogen in Si are also close to each other. The similarity of C and Si properties was reported in [2].

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