Simulation of Transient Enhanced Diffusion of Boron Induced by Silicon Self-Implantation

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Abstract—The time, dose, and energy dependence of boron transient enhanced diffusion (TED) induced by silicon self-implantation has been simulated taking into account the time evolution of self-interstitial clusters. The kinetics of cluster dissolution and growth are combined with the kick-out mechanism for boron diffusion, and the decrease in the cluster evolution rate with time is taken into account. Using a unified set of parameters, the simulation explains some complex characteristics of TED; that is, the enhancement is independent of the implant dose at short annealing times, while it increases with increasing implant dose after longer annealing times. In addition, the implant energy dependence of TED can be explained by the proximity of the damage to the surface.

I. INTRODUCTION

The transient enhanced diffusion (TED) of dopants in silicon is a central issue in silicon device processing [1-4] because TED is a limiting factor for shallow junction formation. It is generally accepted that the large supersaturation of silicon self-interstitials produced by ion implantation damage causes TED. A recent study showed that {311} self-interstitial clusters are the source of the self-interstitials for TED [1], and a kinetic equation has been proposed to describe the time evolution of the cluster [2]. However, to the author's knowledge, there have been no simulation results that quantitatively fit the time dependent profiles of TED, mainly due to the difficulty in modeling the cluster evolution because of the need to take into account the decrease in the evolution rate with elapsed time as small clusters grow into larger ones (Ostwald ripening) [2]. This paper describes a simulation based on the cluster evolution and the kick-out mechanism for B diffusion and that takes into account the decrease in cluster evolution rate with time due to Ostwald ripening. The time evolution of the experimental B TED data induced by Si implantation with different doses and energy [3,4] was successfully fitted using a unified set of parameters.

II. MODEL AND RESULTS

We simulate the B TED profiles according to the kick-out reaction, which includes substituted dopants (B_s), dopant interstitials (B_i), and self-interstitials (I): $B_i \Leftrightarrow B_s + I$ [5]. This reaction together with a kinetic equation to describe the time evolution of the self-interstitial cluster [2] leads to the set of coupled partial differential equations:

$$\frac{\partial C_s}{\partial t} = k_{1f}C_i - k_{1b}C_sC_I \tag{1}$$

$$\frac{\partial C_i}{\partial t} = \frac{\partial}{\partial x}\left(D_i\frac{\partial C_i}{\partial x}\right) - \frac{\partial C_s}{\partial t} \tag{2}$$

$$\frac{\partial C_I}{\partial t} = \frac{\partial}{\partial x}\left(D_I\frac{\partial C_I}{\partial x}\right) + \frac{\partial C_s}{\partial t} - \left(k_fC_IC_c - k_bC_c\right) \tag{3}$$

$$\frac{\partial C_c}{\partial t} = k_fC_IC_c - k_bC_c\ , \tag{4}$$

where C_x (x=s, i, I, and c, respectively for B_s, B_i, free I, and I trapped in the clusters) is the concentration of x, D_x is the diffusivity of x, and k_1 is the rate constant of the kick-out reaction with f and b denoting forward and the backward reactions. In (3) and (4), k_f and k_b denote the rate constants of the cluster growth and dissolution, respectively. Equation (4) was proposed to simulate cluster evolution [2]; however, Ostwald ripening was not included.

In order to describe the decrease in the cluster evolution rate with time due to Ostwald ripening, we assume $k_f=-at+b$ and $k_b=k_fC_{I(*)}$ with a, b, $C_{I(*)}$, and k_b at the second stage being parameters, as will be described below. B diffusion is primarily determined by $D_iC_{i(eq)}/C_s$ and $D_IC_{I(eq)}$ [5], and reported diffusivities [6,7] were used. For the initial profile of C_c, a "+1.4" model [8] was used, and self-interstitial concentration was assumed to be the equilibrium value at the Si surface.

Using the above set of parameters and conditions, (1) - (4) were solved numerically by the partial differential equation solver ZOMBIE [9], and we have satisfactorily fitted the B TED profiles with Si implantation doses of $3\mathrm{x}10^{13}$ and $1\mathrm{x}10^{14}$ cm^{-2} at 50 keV followed by 750 °C annealing [3,4], as shown in Figs. 1 and 2. The following parameter values were used for the simulation: $C_{I(*)}=4.0\mathrm{x}10^{13}$ (cm^{-3}), $a=1.0\mathrm{x}10^{-17}$ (cm^{3}s^{-2}), $b=9.0\mathrm{x}10^{-16}$ (cm^{3}s^{-1}), and $k_b=4.0\mathrm{x}10^{-4}$ (s^{-1}). Note that exactly the same set of parameters were used for both doses. Once the values of $D_iC_{i(eq)}/C_s$ and $D_IC_{I(eq)}$ are fixed, the calculated B profiles become fairly insensitive to the variations of the values of individual parameters D_i and D_I, and $C_{i(eq)}/C_s$ and $C_{I(eq)}$ as long as $C_{I(*)}/C_{I(eq)}$ is fixed. Fig. 3 shows the initial profiles

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used for the simulation, and profiles of the species that were simulated for the 1 min-profile with $3x10^{13}$ cm^{-2} (Fig. 1).

III. DISCUSSION

A. Time Dependence

The time dependence of C_I and C_C at the depth of 0.1 μm deduced from the simulation are shown in Fig. 4 together with that of the k_f used for the simulation, where k_f at the first stage ($\lesssim$ 100s) and k_b at the second stage ($\gtrsim$ 100s) are the essential parameter for each stage. The evolution of TED consists of two time stages, where two contributions are the critical factors; cluster growth, $k_f C_I C_C$, and the self-interstitial diffusion, $D_I(d^2C_I/dx^2)$. At the first stage, where the self-interstitial diffusion away from the Si implanted region is slower than the rate at which the cluster can trap the self-interstitials to maintain the equilibrium concentration of self-interstitials at a constant value $C_{I(*)}$ ($k_f C_I C_C > D_I(d^2C_I/dx^2)$), a pseudo-equilibrium state develops, and $dC_I/dt \approx 0$ and $dC_C/dt \approx D_I(d^2C_I/dx^2)$ hold. Therefore, the self-interstitial diffusion is the rate-determining step for this stage, and $C_{I(*)}$ is determined by the balance between the cluster growth and dissolution. The self-interstitial supersaturation $C_{I(*)}/C_{I(eq)}$ is approximately the enhancement of B diffusivity. In this stage, C_I, and hence the B diffusion enhancement is almost constant with time.

With the elapse of time during the pseudo-equilibrium period, the cluster evolution rates k_f and k_b will slow down due to Ostwald ripening. And finally when $k_f C_I C_C < D_I(d^2C_I/dx^2)$ holds, the cluster cannot maintain the $C_{I(*)}$ value anymore, and the C_I decreases abruptly. Then Ostwald ripening will cease, and hence k_f and k_b become constants. This is the second stage, where the cluster dissolution becomes the rate-determining step. At this stage $dC_C/dt = -k_b C_C$ holds, and C_C and C_I show an exponential decay with time because k_b is a constant. The parameter values for the cluster evolution are uniquely determined as follows: a and b are fixed by the profiles for the $3x10^{13}$ cm^{-2} dose because three of these profiles are in the first stage, and k_b is determined by the profiles for $1x10^{14}$ cm^{-2} because all three of these are in the second stage. The first stage has been previously described [2,3]; however, we give further attention to the growth rate and its change with time and to the enhancement at the second stage.

The C_I curves in Fig. 4 clearly show that the exponential time decay of self-interstitials cannot simulate TED and that taking into account cluster evolution with Ostwald ripening is indispensable to correctly predict it. It should be noted that neglecting Ostwald ripening would prevent simulation of the profiles because C_I would decrease to $C_{I(eq)}$ so quickly that the second stage would not exist, leading to almost identical profiles for 30 min and 2 h, which is inconsistent with the experimental results in Fig. 2.

B. Dose and Energy Dependence

At the first stage, C_I, and hence the B diffusion enhancement, is almost independent of the implant dose (Fig. 4). In addition, using the same parameter set, the dose of $2x10^{13}$ cm^{-2} leads to almost the same enhancement as $3x10^{13}$ cm^{-2}, while $1x10^{13}$ cm^{-2} leads to a smaller enhancement than $3x10^{13}$ cm^{-2}, which is consistent with the experimental results [3] and indicates the validity of our simulation. At the second stage, the enhancement, and hence the overall diffusion displacement increases with larger implant dose.

Fig. 5 shows the simulation results for the energy dependence of the B diffusion distance ($(Dt)^{1/2}$) with $5x10^{13}$ cm^{-2} dose versus annealing time. The simulated results satisfactorily fit the experimental data [3]. The simulation was made using exactly the same parameter set as in Figs. 1 and 2. Self-interstitial concentration was assumed to be the equilibrium value at the Si surface, and no effect of dislocations on C_I, which is believed to be important for higher energy implantation, was taken into account in this simulation. The results indicates that the Si surface surely acts to pin point defect concentrations at equilibrium [4,10], and that the energy dependence of TED can be explained solely by the proximity of the damage to the surface in the implantation energy range covered in this simulation.

C. Cluster Evolution

We have assumed that k_f is described as $-at+b$. Note that k_f should decrease with time, otherwise free self-interstitials resulting from cluster dissolution would be trapped again by the cluster before they could diffuse away, and the first stage of TED would be much longer than shown in Fig. 4, which leads to overestimating the B displacement after about 100 s. We attribute this decrease in k_f to the decrease in the effective C_C because free self-interstitials may be less likely to be trapped by the clusters as they grow larger and the cluster density decreases. This model seems reasonable because the cluster size appears to be independent of dose; only their density differs with different doses [3]. Note that k_f is time dependent only in the first stage, and hence is independent of C_I because $C_I \approx C_{I(*)}$ holds at the first stage.

Dividing the total self-interstitial concentration in the cluster by the cluster density [1], the time dependence of the number of self-interstitials per cluster during Ostwald ripening can be fitted by $1/(-at+b)$, as shown in Fig. 6 Because only data at 815 °C are available and the kinetics of Ostwald ripening for the {311} clusters are not well understood, we also used this relation for 750 °C, and we

have satisfactorily fitted the B TED profiles (Figs. 1 and 2), which indicates that the above assumption is reasonable.

Concerning the temperature dependence of k_f, a and b should have the dependence with the activation energy of the cluster growth rate. In addition to this temperature dependence, because k_f is proportional to the effective C_c, a increases with higher temperature due to faster Ostwald ripening, and b decreases due to the possible increase in the initial cluster size (at t=0), resulting in smaller effective C_c. Because the kinetics of the {311} clusters and of the Ostwald ripening are not well understood, the experimental data for other temperatures are required in order to evaluate the temperature dependence of a and b. The variation of implantation species has no significant effect on the enhancement in TED [11], which is related to the cluster size [3], and hence to the effective C_c. This suggests that k_f is also independent of implantation species at a given temperature.

IV. CONCLUSIONS

The time, dose, and energy dependence of boron TED induced by silicon self-implantation has been simulated using parameters that correspond to the equilibrium self-interstitial concentration under the equilibrium between the clusters and free self-interstitials, the time dependent rates for cluster evolution, as well as the fluxes of boron interstitials and self-interstitials. The simulation results fit reported experimental profiles and correctly predict the time, dose, and energy dependence of the TED. Since this study clarifies the essential parameters for determining the time dependence of the self-interstitial behavior that governs TED, it is widely applicable to the TED induced by other implants.

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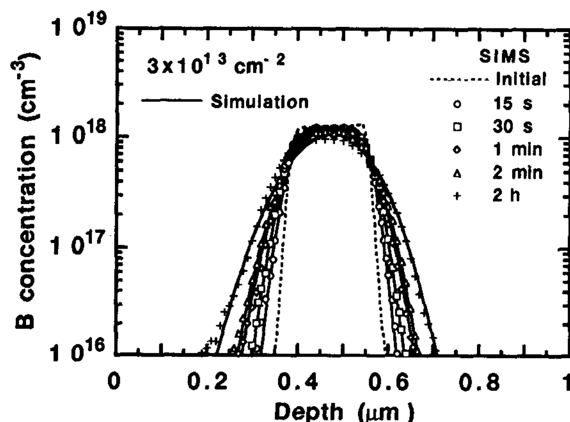

Fig. 1 Simulated (solid lines) and SIMS (symbols: [3]) B profiles with 50 keV, 3×10^{13} cm^{-2} Si implantation and annealing at 750 °C.

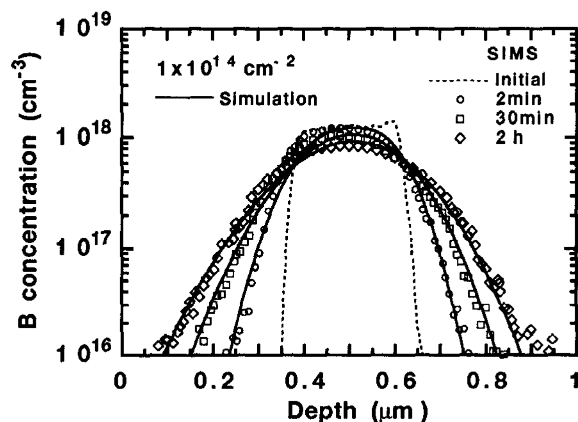

Fig. 2 Simulated (solid lines) and SIMS (symbols: [4]) B profiles with 50 keV, 1×10^{14} cm^{-2} Si implantation and annealing at 750 °C.

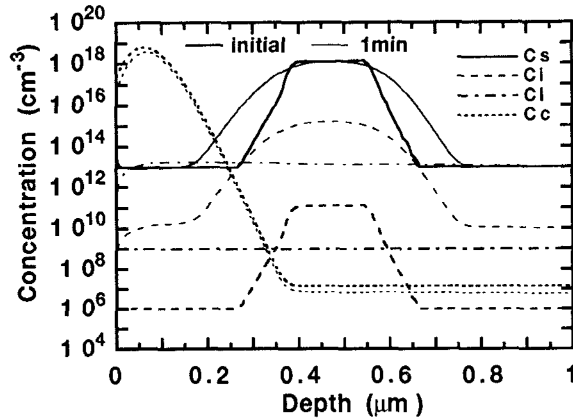

Fig. 3 Initial profiles used for the simulation, and profiles of the species that were simulated for the 1 min-profile with $3x10^{13}$ cm^{-2}.

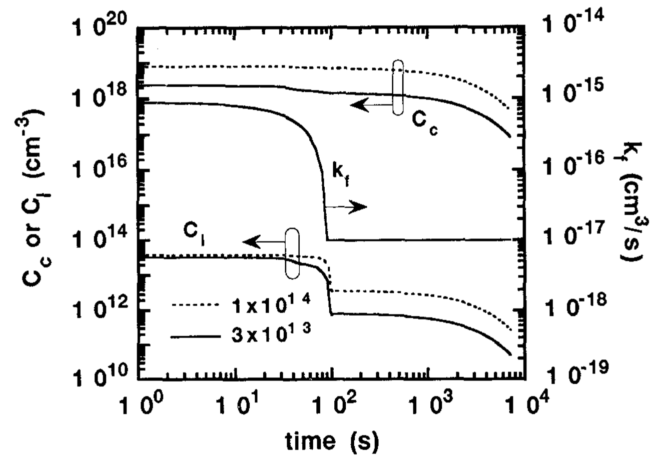

Fig. 4 The time dependence of C_I and C_c at the depth of 0.1 μm deduced from the simulation together with that of k_f used for the simulation. The lower limit of $k_f=-at+b$ is $k_b/C_I(*)>0$. $C_I=1x10^{13}$ cm^{-3} corresponds to B diffusion enhancement $C_I/C_I(eq)$ of 10^4 because $C_I(eq)= 1x10^9$ cm^{-3} was used.

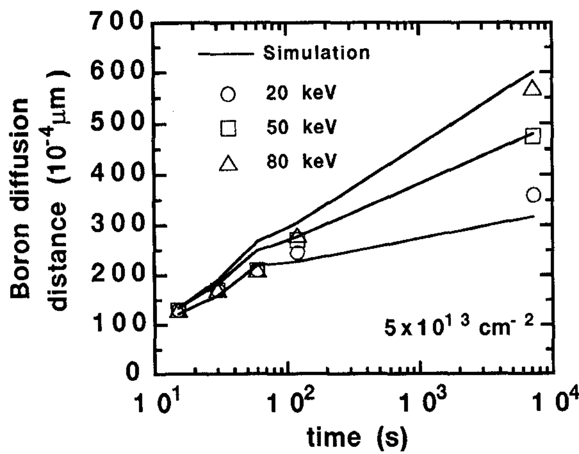

Fig. 5 Simulated results for the energy dependence of the B diffusion distance with $5x10^{13}$ cm^{-2} dose. Experimental data are from [3].

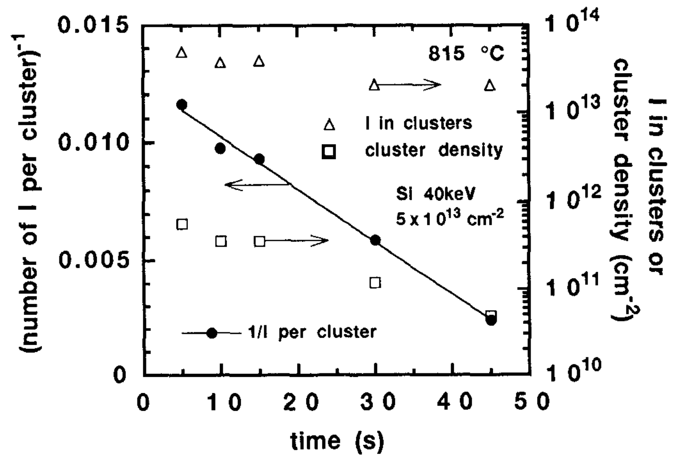

Fig. 6 The reciprocal of the number of self-interstitials per cluster during Ostwald ripening can be fitted by $-at+b$. Dividing the cluster density by the total self-interstitial concentration in the cluster [1] gives the reciprocal values. The reciprocal values are plotted to show the linearity.