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TED Model Including the Dissolution of Extended Defects

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1. Introduction

The requirement for the formation of the shallow junction has arisen as device dimensions shrink into the submicron regime. The shallow junctions are generally formed by low-energy ion implantation followed by low thermal-budget processing. However, simulations of dopant diffusion during the thermal processing have not been very successful, mainly due to the transient enhance diffusion (TED). TED continues until the concentrations of the point defects, interstitial silicon, and vacancies become almost their thermal equilibrium values. In an earlier model, the defect concentrations decrease through diffusion and recombination [1]. However, Michel showed experimentally that the activation energy of TED saturation is 4.3eV [2], which is larger than that of diffusion and recombination of the defects. Fig. 1 illustrates the activation energy of the dissolution of the extended defect, a dislocation loop [3]. The activation energy of this phenomena is almost the same as that of the TED saturation. Kim et al. showed experimentally that TED saturates when the dislocation loop disappears [4]. In addition, Liu et al. experimentally indicate the extended defects, a dislocation loop, dissolve during the annealing, resulting in the emission of the free interstitial silicon [5]. For accurate simulation of TED, the effect of the extended defect dissolution cannot be neglected. In this work, we propose a new TED model which includes the extended defect dissolution.

2. TED model including the extended defect dissolution

Our model for TED is based on the non-equilibrium point defect model [6]. The impurity diffuses through the E-center and kick-out mechanism which are mediated by the vacancy and the interstitial silicon, respectively. To include the effect of the extended defect dissolution, the diffusion equation for the interstitial silicon is changed to the following equation,

$$\begin{aligned}\frac{\partial C_I}{\partial t} &= \frac{\partial}{\partial r}\left(D_I \frac{\partial}{\partial r} C_I\right)\\ &- k_{bi}\left(C_V C_I - C_V^{eq} C_I^{eq}\right) + \sum_D \left(k_{DI}^r C_{DI} - k_{DI}^f C_{D+} C_{I-}\right) + \sum_A \left(k_{AI}^r C_{AI} - k_{AI}^f C_{A-} C_{I+}\right),\\ &+ k_{ed} C_{ed}\end{aligned} \quad (1)$$

where C is the concentration, D is the diffusion constant, and k is the reaction constant. The subscripts I, V, D, A, and ed represent the interstitial silicon, vacancy, donor, acceptor and the extended defect, respectively. The superscripts eq, r, and f represent the equilibrium condition, and the reverse and forward reactions, respectively. The last term on the right side of Eq. (1) expresses the effect of the extended defect dissolution. The dissolution rate, k_{ed}, is

$$k_{ed} = k_{ed0} \exp\left(-E_{k_{ed}} / kT\right) \quad (2)$$

The initial concentration of the captured silicon atoms in the extended defects, $C_{ed,0}$, is defined by,

$$C_{ed,0} = C_{I0}\theta(C_{I0} - C_{I,\min})\theta(C_{I,\max} - C_{I,0}), \quad (3)$$

where C_{I0} is the initial concentration of interstitial silicon, and θ is the θ -function. The values of $C_{I,max}$ and $C_{I,min}$ are determined empirically to be 1×10^{21}cm^{-3} and the intrinsic carrier concentration, respectively. The extended defect has been known to grow through the coarsening and dissolution regime [5]. Eq. (1) and Eq. (2) neglect the coarsening regime. Although the extended defects of earlier work are modeled to behave as the absorber of interstitial silicon after the ion implantation [7], this work models extended defects as the emitter of the interstitial silicon from the beginning of the annealing (Fig. 2). Parameters for the extended defect model are listed in Table 1.

3. Simulation results

Figure 3 shows simulation results in which a 1.0×10^{14}cm^{-2} dose of phosphorus is implanted into a silicon substrate at 40 keV followed by the 850℃ annealing for 1min. In this figure, the profile of the interstitial silicon is made up of the free interstitial silicon and the extended defect. The extended defects gradually emit the free interstitial silicon. To verify the accuracy of our model, we compared ΔX_j dependency on the annealing time of the simulation and experimental results. Here, ΔX_j is defined by the depth difference between the points where the concentration of doped impurities is 1×10^{17} cm^{-3} before and after the annealing. Good agreement is obtained, as shown in Fig. 4.

References
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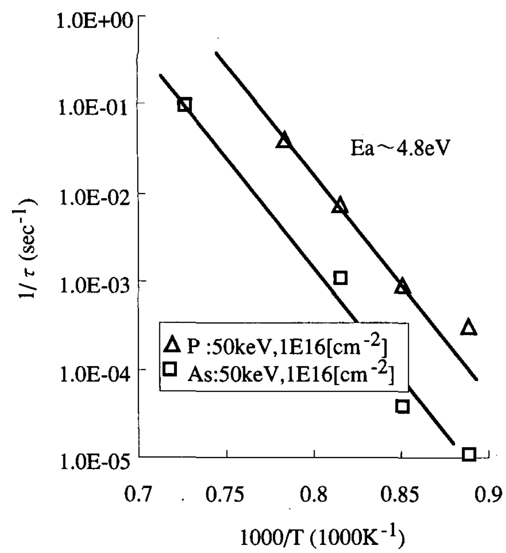

Fig. 1. Arrhenius plot of the dissolution time of the extended defects (dislocation loop)[3].
The activation energy is almost the sameas that of the TED saturation time.

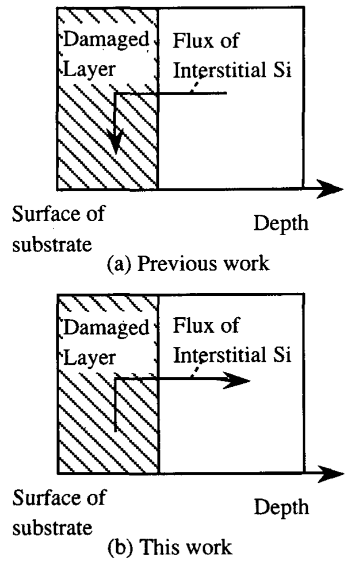

Fig. 2. Comparison between the previous work [8] and this work. The previous work introduced the extended defect to explain the saturation of the oxidation enhance diffusion.

Table 1 Parameters for the extended defect model.

Parameter	B	P	As	Sb
g_{RP0} (cm/s)	8.66E-7	8.66E-7	8.66E-7	8.66E-7
E_{RP} (eV)	1.0	1.0	1.0	1.0
g_{nL0} (/s)	3.0E+17	1.0E+17	1.0E+16	1.0E+16
E_{nL} (eV)	4.4	4.4	4.4	4.4

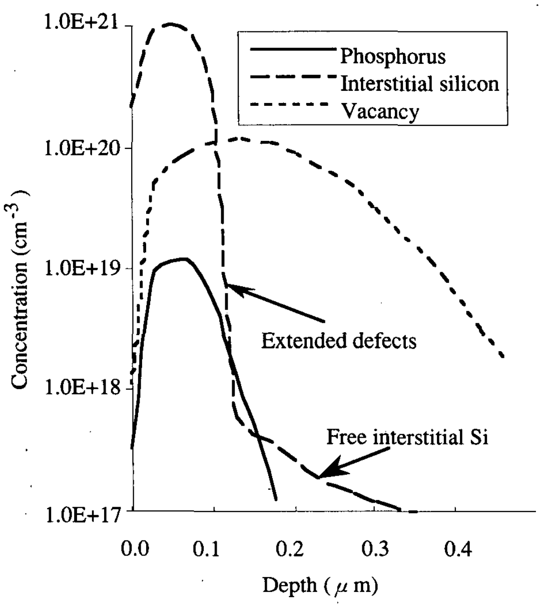

Fig. 3. Simulated profile of the interstitial silicon, vacancies, and phosphorus. The profile of the interstitial silicon is made up of the extended defects and the free interstitial silicon.

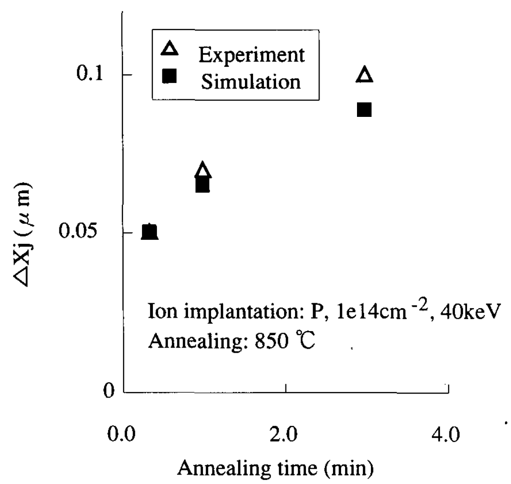

Fig.4. Comparison of △Xj dependency on the annealing time between the simulation and the experimental results.