KMC Simple Model for B_mI_n Cluster Evolution during Boron Diffusion : Theoretical or Experimental Parameters of Point Defects

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ABSTRACT

In this paper, we investigate the simple model for the explanation of the evolution of interstitial clusters during boron diffusion for implementing the kinetic Monte Carlo (KMC) code. It is well understood that posterior to the ion implantation some clusters play a decisive role for the enhanced boron diffusion at the tail region while immobile at the peak region. Our model, which is based on the simple continuum theory convenient for implementing the kMC code, considers the intermediate clusters as well as definite dominant clusters for building the evolutionary behavior of interstitial clusters during boron diffusion. We found out that the intermediate clusters such as B_3I_3 and B_3I_2 play a significant role during the evolution of clusters because the lifetimes of the corresponding intermediate clusters are relatively short due to low binding energies. Additionally, we confirm that B_3I is the most dominant cluster after annealing. Also, we use a simple model [1] adopted kMC method to investigate the KMC parameters of for interstitial, vacancy and B_mI clusters based on theoretical calculation and experimental data during boron diffusion. Finally, our model was verified with experimental SIMS data, which supports our theory that intermediate interstitial clusters and the parameters are very important in the atomistic model in order to understand the whole diffusion process of boron in silicon.

Keywords: atomistic simple model, Kinetic Monte Carlo, Boron diffusion,

1 INTRODUCTION

For modeling and simulation for diffusion of impurities in silicon crystal, there have been used two kinds of mathematical approaches. The one approach is the continuum model which employs a deterministic method such as finite difference method or finite element method. These methods have been applied to various branches of science and engineering. Recently, a simple continuum model composed of dominant clusters has been introduced to model the full continuum model. The other model is atomistic model such as kinetic Monte Carlo method. The above-mentioned KMC is based on Poisson process combined with Monte Carlo approach. The continuum model has been considered to be tolerably accurate for explaining the diffusion process in submicron regime. However, the accuracy becomes poor and poor as the scale of devices goes down into nanometer regime. We propose a new atomistic model composed of dominant clusters and intermediate clusters to realize the complicated diffusion process, which can be easily implemented in the atomistic approach.

In additional research, we also present the investigation of KMC parameters for interstitial, vacancy and B_mI_n clusters during annealing. The parameters for interstitial and vacancy are calculated theoretically [6] or are extracted from experiments [7]. The parameters are important to determine the accuracy of results of simulation. Until now, either the theoretical parameters or the experimental parameters have been used in modeling. However, the accuracy of model using such parameters differs as the scale of devices goes down into nanometer scale. The simple atomistic model based on a simple continuum model simply adds some other clusters such as B_3I_3, B_2I_3 to the continuum model because of finding out that the simple continuum model is not in accordance with SIMS data. B_3I_3 and B_2I_3 play an important role to build dominant clusters in our model. We apply the parameters to the simple atomistic model to show that the theoretical parameters are plausible than the experimental ones in KMC and demonstrate our simple atomistic model and further compare our model with experimental SIMS profile as well as the conventional continuum model.

2 KINETIC MONTE CARLO IMPLEMENTATION

In KMC, a physical system which consists of many possible events evolves as a series of independent events occurring. All events have their own the event rates. Event rates are calculated by Eq (1). E_b is the migration-energy barrier for jump events or a binding energy for cluster evaporation. v_0 is the attempt frequency, which is simply the vibration frequency of the atoms. In most cases, it is of the order of 1/1000fs. Theses parameters come from *ab-initio* calculations or experimental data [6, 7]

$$v = v_0 \cdot E^{(\frac{E_b}{K_B T})} \quad (1)$$

Here, k and T represent Boltzman's constant and temperature respectively. We consider thermally activated events in the thermal annealing simulation after ion implantation. If the probability for the next event to occur is independent of the previous history, and the same at all times, the transition probability is constant. Then, the process is a so-called Poisson process. To derive the time dependence, consider a single event with a uniform transition probability r [7]. Let f be the transition probability density, which gives the probability rate at which the transition occurs at the time t. The change of $f(t)$ over some short time interval dt is proportional to r, dt and f, because f gives the probability density that the physical, system still remains at time t,

$$df(t) = -rf(t)dt \quad (2)$$

Further, the solution is given by with boundary conditions,

$$f(t) = re^{-rt}, f(0) = r \quad (3)$$

Therefore, the simulation time is updated for ($t = t + \Delta t$) according to event rates as follows, because an ensemble of independent *Poisson process*:

$$\Delta t = -\frac{\ln u}{R} \quad (4)$$

Here, u is a random number and R is the total sum of all possible events rates. Therefore KMC is suitable to simulate non-uniform time evolution process.

3 ATOMISTIC SIMPLE MODEL

The title basically, the simple atomistic model uses interstitialcy mechanism that dopants diffuse in the form of the mobile defect, BI. Later, the defect forms extended defects by encountering other defects. Thereafter, the extended defects play an important role of boron diffusion. In our simple atomistic model, we find that the results of simple atomistic model including only clusters used in the simple continuum model are not in accordance with the SIMS data. So, we add some cluster models in simple continuum model for the accuracy of simple atomistic model.

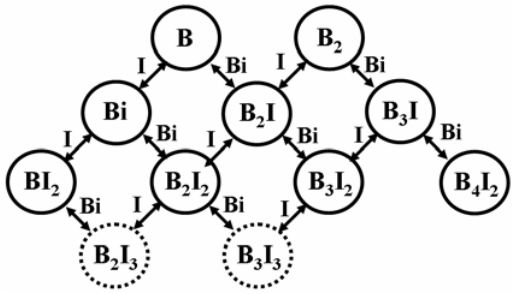

Figure1. Supplemented clusters (dotted line) in simple model [1].

Figure 1, we propose that BI_2 would evolve to B_2I_3 or BI and B_2I_2 to B_2I or B_3I_3. Namely, we find that B_2I_3 and B_3I_3 play a special role in the evolution of dominant clusters.

$$B_s + I \Leftrightarrow B_i \quad (5)$$

$$B_m I_n + I \Leftrightarrow B_m I_{n+1} \quad (6)$$

$$B_m I_n + B_i \Leftrightarrow B_{m+1} I_{m+1} \quad (7)$$

We demonstrate the simple atomistic model. So, we add the other clusters such as B_2I_2 and B_3I_2 to the simple continuum model. The evolution of clusters progress by equation (5, 6).

3 SIMULATION RESULTS AND DISCUSSION

We pick up dominant clusters among many clusters throughout cluster data and confirm the number of dominant clusters formed during thermal annealing. Figure 2 shows the number of dominant clusters formed during thermal annealing. In implantation and initial annealing, because the event rate of interstitial is high, first BI is created, and then BI_2 becomes a dominant cluster while the

other defects recombine and form the extended defects. However, B_3I becomes the most dominant cluster within a second.

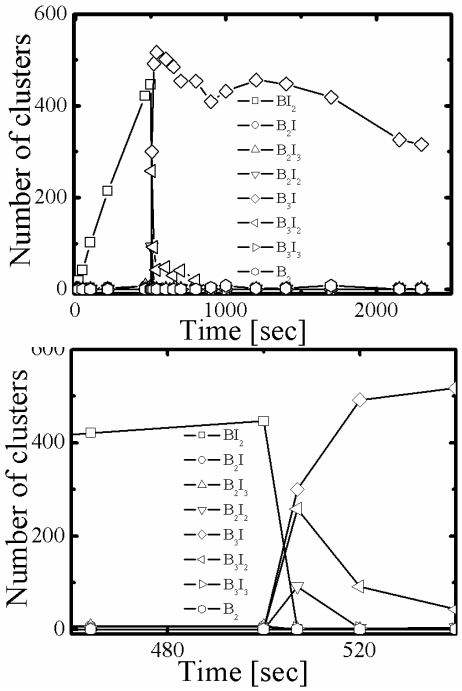

FIG. 2. Number of clusters versus time for 5 x 10^{14}cm^{-3}, 20keV boron implant, after a 30min anneal at 800℃.

Figure 1 shows schematically dominant clusters and intermediate clusters. Intermediate clusters impacting the evolution of dominant clusters are small in number as shown in Fig. 2. However, those clusters play an important role in the evolution of clusters. It is noted that the lifetimes of the intermediate clusters are short due to low binding energies. In figure 3 and 4, the model parameters of the simple atomistic model use theoretical and experimental total binding energies that are needed to break up clusters and to migrate separated mobile defects. Figure 5 is the boron profile of boron of 5 x 10^{14}cm^{-2}, 20 keV, (a), 800℃, for 30 min (b) 800℃,for 2 h (c) 900℃, for 30 s and (d) 2 x 10^{14}cm^{-2}, 800℃, for 1 h in the simple atomistic and the simple continuum models. Figure 6 shows the boron profiles with the parameters in the simple atomistic model. As the amount of dose goes up, the boron profiles respectively with the parameters are different in tail. Figure 3 shows the KMC parameters for interstitial and vacancy. In conclusion, we extract a dominant B_mI_n complex profile including B_3I, B_3I_3 and B_2I_2 cluster and confirm the distribution of boron in the simple atomistic model in Figs. 2 and 5.

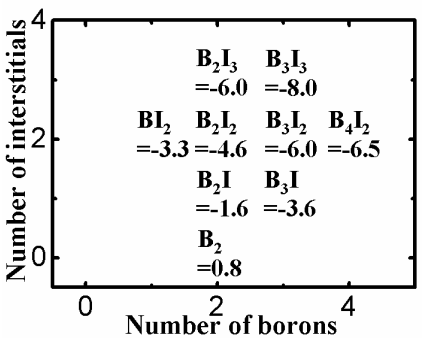

FIG. 3. Total binding energies [6, 7].

Experimental parameters	Theoretical parameters
Interstitial	Interstitial
D_i= 2 cm^2/sec E_m= 0.9 eV	D_i= 5 x 10^{-3} cm^2/sec E_m= 1.0 eV
Vacancy	Vacancy
D_v= 5 x 10^{-6} cm^2/sec E_m= 0.43 eV	D_v= 1 x 10^{-3} cm^2/sec E_m= 0.4 eV

FIG. 4. The parameters used in simple atomistic model, [6, 7].

4 CONCLUSION

In this paper, we report the role of clusters in the atomistic process for the implementation into KMC and compared our simulation with the experimental SIMS data. Our model implies that that B_3I is the most significant cluster in boron diffusion posterior to annealing. We found out that all kinds of intermediate clusters should be taken into account for an accurate KMC calculation and that distribution of boron in the diffusion process can be simulated with the simple atomistic model.

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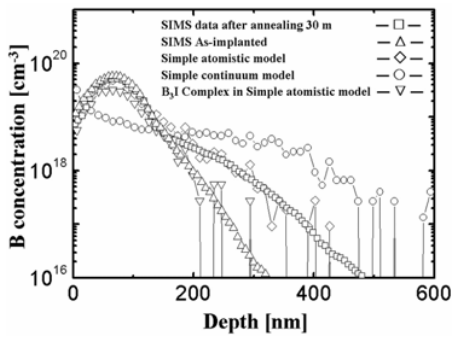

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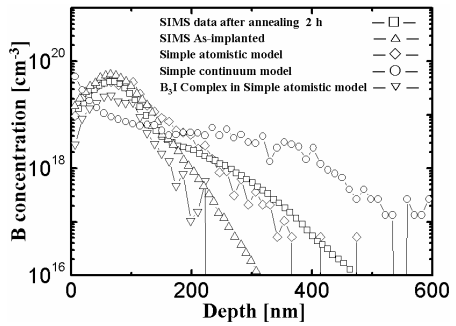

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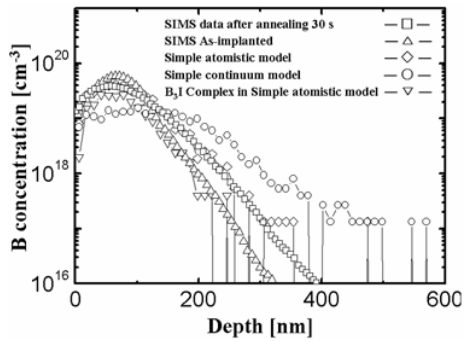

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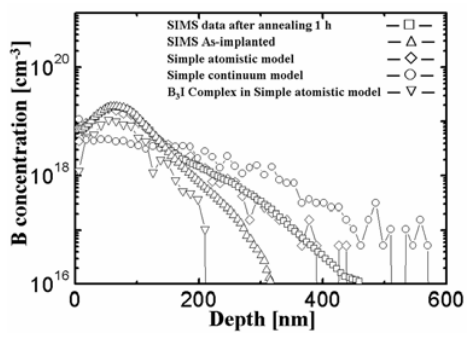

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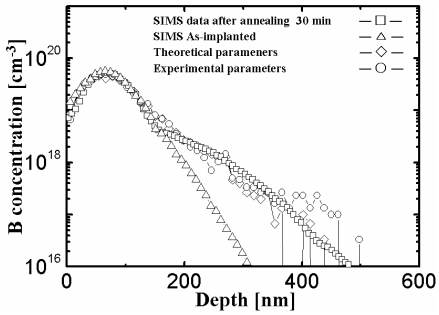
FIG. 5. Comparison of simple Atomistic model to SIMS and simple continuum model data for boron of 5 x 10^{14}cm^{-2}, 20 keV, (a), 800℃, for 30 min (b) 800℃,for 2 h (c) 900℃, for 30 s and (d) 2 x 10^{14}cm^{-2}, 800℃, for 1 h. SIMS is calculated by M. D. Giles and S. Slomi, et al., [3] [4].



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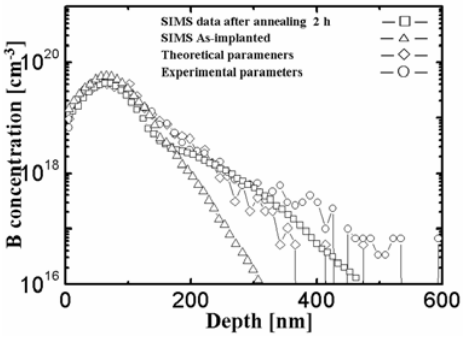

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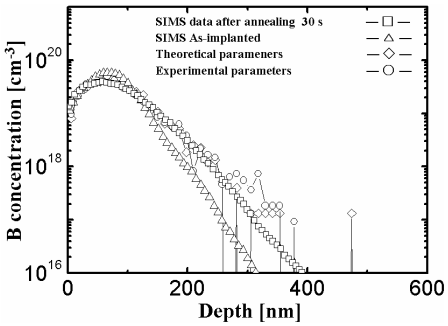

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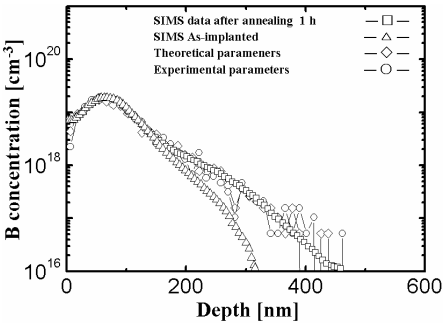

(d)

FIG. 6. Comparison of simple atomistic model with the parameters for boron of 5 x 10^{14}cm^{-2}, 20 keV, (a), 800℃, for 30 min (b) 800℃,for 2 h (c) 900℃, for 30 s and (d) 2 x 10^{14}cm^{-2}, 800℃, for 1 h. SIMS is calculated by M. D. Giles and S. Slomi, et al., [3] [4].