Kinetic Monte Carlo Modeling of Boron Diffusion in Si Crystalline Materials

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ABSTRACT

In this paper, we report a lattice-free kinetic Monte Carlo (KMC) result of boron diffusion at low temperatures 450℃ and 550℃ with vacancy + interstitialcy mechanism or vacancy + kick-out one with dilute self-interstitials (I) and vacancies (V) created in a B-doped marker layer (4×10^{11}B/cm^2 per marker) by Si implantation (50keV, 10^{11}/cm^2). In this type of KMC model, point defects and dopants are treated at an atomic scale while they are considered to diffuse in accordance with their event rates, which are given as input parameters from *ab initio* calculations or experimental data. Especially, the formation of clusters and extended defects, which usually control the annealing kinetics after ion implantation, is to be minimized in the range of low doses in an effort to create dilute concentrations of I and V. Therefore, simple vacancy and kick-out or interstitialcy mechanisms without interstitial clusters or extended defects are tested in these conditions and both are in a good agreement with the SIMS data. However, in these dilute concentrations vacancy mechanism plays a dominant role in B diffusion in place of the usual kick-out or interstitialcy mechanism in boron enhanced diffusion.

Keywords: Atomistic diffusion modeling and simulation, kinetic Monte Carlo, Boron diffusion, Interstitialcy mechanism, Kick-out mechanism.

1 INTRODUCTION

In nano-scale semiconductor process simulation, an atomic scale model is essential because of the destined failure of continuum approach in small nano scales. Molecular dynamics (MD), the most in-detailed description at an atomic level is not adequate in thermal annealing simulations after ion implantation due to that MD can not span the long time of thermal annealing. Therefore, kinetic Monte Carlo (KMC) method for simulating the thermal annealing has been preferred.

In this paper, we report a model for diffusion of Boron at low temperatures with vacancy and interstitialcy or kick-out mechanism [4,6,7] with Si self-interstitials (I) and vacancies (V) created in a B-doped marker layer by Si implantation [3]. For an accurate atomic-scale model for diffusion of intrinsic point defects (I, V) and impurities (B) in ion-implanted silicon, we use a lattice-free KMC method. In this type of KMC model, point defects and dopants are treated at an atomic scale while they are considered to diffuse in accordance with their event rates, which are given as input parameters from *ab initio* calculations or experimental data. Especially, the formation of clusters and extended defects, which usually control the annealing kinetics after ion implantation, is minimized in the range of low doses to create dilute concentrations of I and V. In these conditions, the formation of clusters and extended defects are ignored to study only boron diffusion mechanisms.

2 KINETIC MONTE CARLO IMPLEMENTATION

In KMC, a physical system, which consists of many possible events, evolves as a series of independent event occurrings. All events have their own event rates. We consider thermally activated events in thermal annealing simulation after ion implantation. If the probability of next event to occur is independent of the previous history, and the same at all times. The transition probability is a 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. Let f the transition probability density, which gives the probability rate at which the transition occurs at 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.

$$df(t) = -rf(t)dt \tag{1}$$

And the solution is given by with boundary conditions.

$$f(t) = re^{-rt}, f(0) = r \tag{2}$$

Therefore, we update the simulation time with ($t = t + \Delta t$) according to event rates as follows because an ensemble of independent Poisson processes will behave as one large Poisson process:

$$\Delta t = -\frac{\ln u}{R} \tag{3}$$

Here, u is the random number and R the total sum of all possible event rates. We select an event according to the

event rates and KMC is proper to simulate non-uniform time evolution processes.

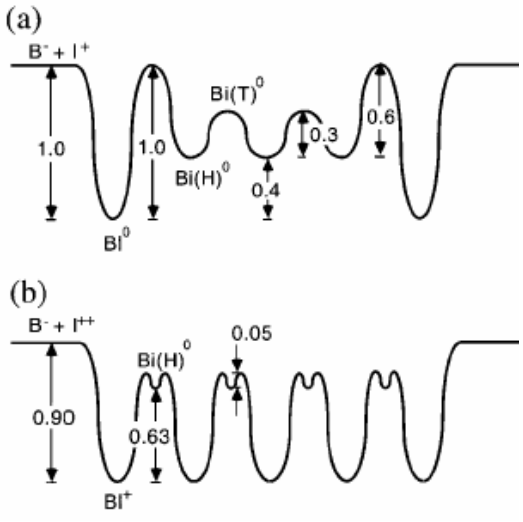


Figure 1: Boron diffusion paths and energy barriers taken from [6], (a) kick-out mechanism and (b) interstitialcy mechanism.

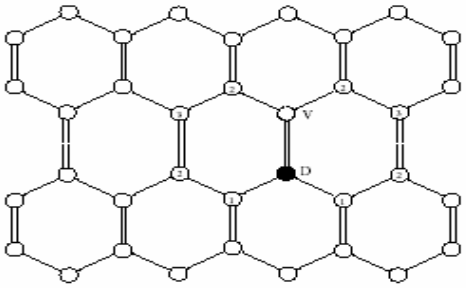


Figure 2: Boron vacancy diffusion mechanism taken from [8] : The vacancy can go around the six member ring of atoms and approach the dopant from a different direction. After the dopant hops into the now empty site the dopant vacancy pair completes one diffusion step.

We implement an atomistic diffusion mechanism involving fast-migrating intermediate species of the form. The reactions $X_s + V \Leftrightarrow XV_m$, $X_s + I \Leftrightarrow X_m$,and $I + V \Leftrightarrow 0$ are essentially diffusion limited, with capture radius of second neighbor atomic length (3.84Å) and direction of particle migration is limited to six neighboring sites. Here X_s is the immobile substitution impurity, which through reaction with a vacancy or a Si self-interstitial (I) forms a fast-migrating species XV_m and X_m, which diffuse at a rate D_m. Ordinary, the diffusion rate is in Arrhenius form ($D_0 \exp(-E_b/kT)$). A simulation box of 1000×1000×2500 $Å^3$ (about 120 (B), 750 (I, V) particles) is used. The width of the simulation box is much smaller than that of the implantation window. Thus, the periodic boundary condition is applied to the box in the lateral direction. Figure 1 shows the Boron diffusion paths and energy barriers of kick-out and interstitialcy mechanisms. Figure 2 shows Boron vacancy diffusion mechanism (ring mechanism) [8]. In addition, all the necessary reactions and parameters are given in Table 1 and Table 2.

Table 1 : Reaction equations

Common diffusion mechanism	
$I + V \Leftrightarrow 0$ $Bs + V \Leftrightarrow BV$	
Interstitialcy mechanism	Kick-out mechanism
$Bs + I \Leftrightarrow BI$	$Bs + I \Leftrightarrow BI$ $BI \Leftrightarrow Bi$

Table 2 : Parameters for simulation [9], [10].

Events	V_0 (10^{15}/s)	E_b (eV)
I migration	0.1	0.9
V migration	0.0025	0.43
BI migration	0.1	0.68
BI → B + I	0.01	0.9
BV migration	0.01	1.0
BV → B + V	0.01	0.5

3 SIMULATION RESULTS

Figure 3 (a) and (b) show boron dopant profiles in MBE-grown marker layer with of about 7 nm (4×10^{11}B/cm^2 per marker) modified by 50 keV Si ion implantation with the dose of $1\times10^{11}/cm^2$ using MARLOWE code. The white circles represent the initial distribution of boron and the black circles the distribution of boron after the thermal annealing for 15 min at 450℃, 550℃, respectively. Figure 5 (a) and (b) shows the boron distribution using vacancy and kick-out mechanism. The two cases of boron diffusion profiles are quite close to SIMS data (asterisk symbols). A significant fraction of B atoms in the shallow marker are displaced and migrate a considerable distance (~10^2 nm) from their initial positions.

In the interstitialcy mechanism, boron with one interstitial (BI) is only mobile species. It can diffuse into silicon lattice via switching BI (tetrahedral sites, T) to Bi (hexagonal sites, H) and Bi to BI. The BI can also break up into substitution B and one mobile interstitial. But, the BI is not mobile particle in kick-out mechanism. In this case, BI can only break up (BI⇔B+I) or kick B out of the silicon lattice (BI⇔Bi, kick-out mechanism). Thus, boron-interstitial (Bi) can diffuse into interstitial sites (H, T).

Figures 4 and 6 represent the time evolution of the number of mobile particles and immobile ones during the thermal annealing. In early stage of diffusion, vacancy mechanism plays a dominant role because of the frequent V migration. The considerable differences are not detected between interstitialcy and kick-out mechanism results in our simulations. These simulation results are caused by the similarity of the total energy barriers between kick-out and interstitialcy mechanisms. In addition, in these dilute concentrations of I and V, the vacancy mechanism plays a dominant role in B enhanced diffusion due to the higher migration frequency of vacancies.

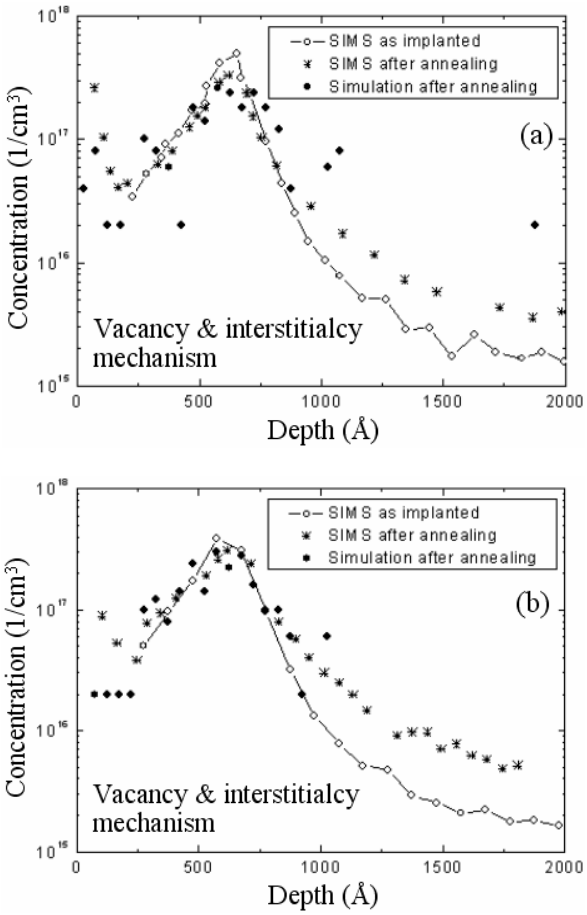


Figure 3: Dopant profiles of MBE-grown boron marker modified by 50 keV Si ion implantation to dose of 1×10^{11} /cm^2 [3] using vacancy and interstitialcy mechanism. (a) 450℃, (b) 550℃ after 15min annealing

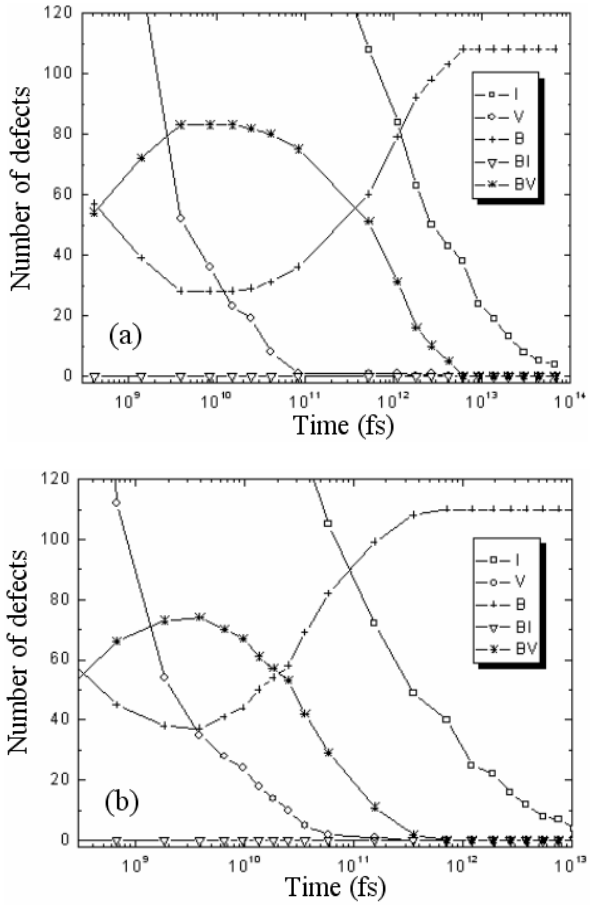
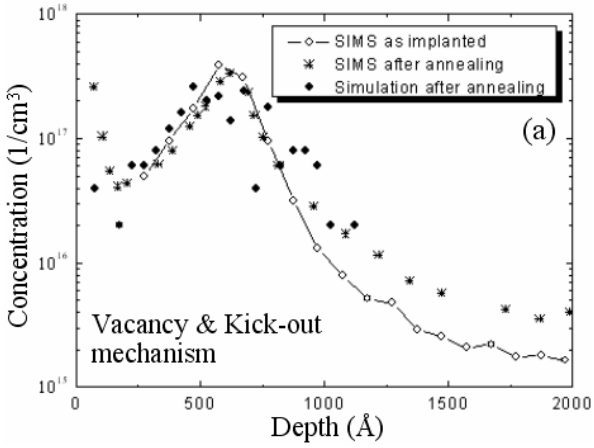


Figure 4: Time evolution of the number of particles in boron MBE-grown marker layer modified by 50 keV Si ion implantation to dose of 1×10^{11} /cm^2 using vacancy and interstitialcy mechanism. (a) 450℃, (b) 550℃ during the annealing



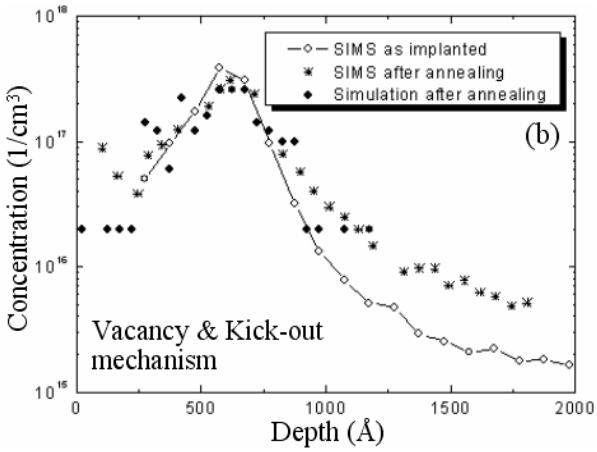


Figure 5: Dopant profiles of boron MBE-grown marker modified by 50 keV Si ion implantation to dose of 1×10^{11} /cm^2 [3] using vacancy and kick-out mechanism. (a) 450℃, (b) 550℃ after 15 min annealing.

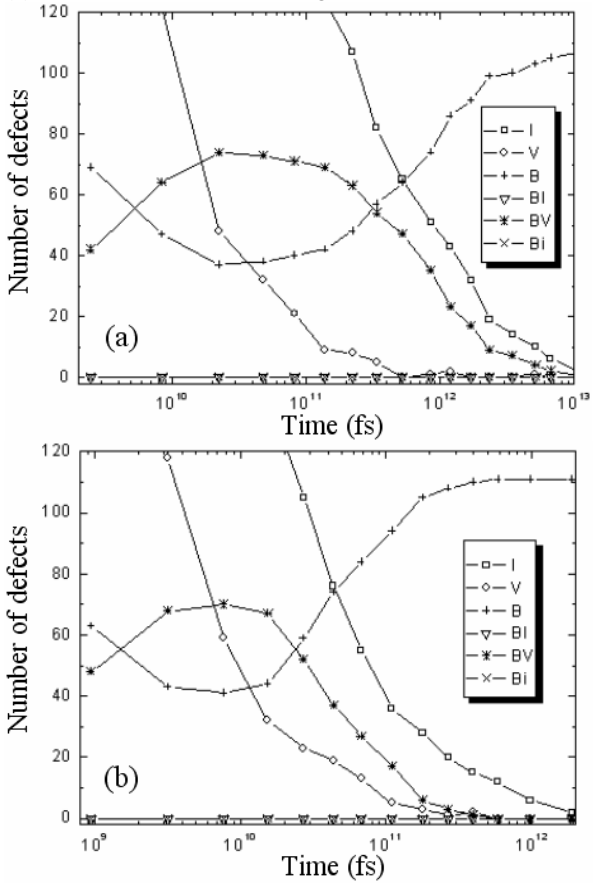


Figure 6: Time evolution of the number of particles in boron MBE-grown marker layer modified by 50 keV Si ion implantation to dose of 1×10^{11} /cm^2 using vacancy and kick-out mechanism. (a) 450℃, (b) 550℃ during the annealing

4 CONCLUSION

In this paper, we implement a KMC simulation for B migration via vacancy and interstitialcy mechanism or kick-out mechanism at low temperatures, 450 and 550℃. Also, to ignore the formation of clusters and extended defects and to study only Boron diffusion mechanisms, low dose experimental data are used.

In our simulations, we find that there is no essential B diffusion difference between vacancy + kick-out and vacancy + interstitialcy mechanisms. This result can be inferred from the fact that the total energy barriers of kick-out and interstitialcy mechanisms are similar. In addition, in these dilute concentrations of I and V, in place of the usual kick-out or interstitialcy mechanism vacancy mechanism plays a dominant role in B diffusion due to the frequent migration of vacancies.

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