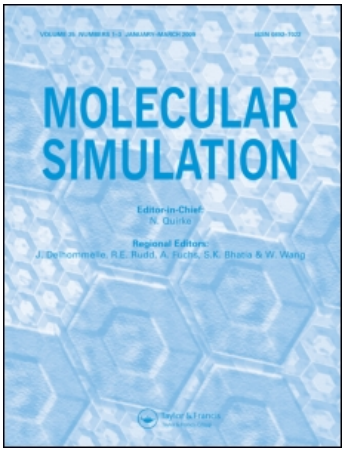

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Simple atomistic modeling of dominant $B_{<i>m</i>}I_{<i>n</i>}$ clusters in boron diffusion

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Simple atomistic modeling of dominant B_mI_n clusters in boron diffusion

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In this paper, we present a simple atomistic model for describing the evolution of interstitial clusters during boron diffusion in kinetic Monte-Carlo (KMC) calculation. It has been known that clusters generated after ion implantation play a decisive role in the enhanced boron diffusion at the tail region while being immobile at the peak region. Our model, which is based on the simple continuum model, takes the intermediate clusters into account as well as dominant clusters for describing the evolutionary behavior of interstitial clusters during boron diffusion. We found that the intermediate clusters such as B_3I_3 and B_2I_3 play a significant role during the evolution of clusters despite the fact that the lifetimes of the corresponding intermediate clusters are relatively short due to low binding energies. Further, our investigation revealed that B_3I is the most dominant cluster after annealing. We applied our simple atomistic model to the study of boron retardation in arsenic pre-doped substrate. KMC simulation results were compared with experimental SIMS data, which supports our theoretical model.

Keywords: Atomistic simple model; Kinetic-Monte Carlo; Boron diffusion; Boron retardation

1. Introduction

In order to model the diffusion process of impurities in silicon crystal, continuum models have been widely employed for up to 100 nm process, which employs deterministic methods such as finite difference method or finite element method. The continuum models are considered to be tolerably accurate for explaining the diffusion process in submicron regime. However, the accuracy becomes poorer as the scale of devices reach nanometer regime.

In this paper, we propose a new atomistic model including dominant clusters and intermediate clusters in an effort to simplify the complicated boron diffusion process. Our model can be easily implemented in the atomistic approach. It was revealed that the simple atomistic model, which is based on the simple continuum model [1], needs some intermediate clusters such as B_3I_3 and B_2I_3. Consequently, we realized that B_3I_3 and B_2I_3 play an important role in building dominant clusters and that B_3I is the most dominant cluster in boron diffusion.

By implementing our simple atomistic model in KMC, we investigated the boron retardation. Boron retardation is known as a phenomenon wherein boron diffusion via interstitial mechanism competes with arsenic diffusion via interstitial and vacancy mechanism in As-doped substrate.

There are some discrepancies between experimental parameters and theoretical *ab initio* ones for interstitial and vacancy [2]. In this paper, we used both parameters to see which parameters are more plausible in the atomistic modeling. From our investigation, the theoretical parameters for interstitial and vacancy in the atomistic process are found more appropriate than the parameters taken from the experimental data.

2. Kinetic Monte Carlo method

Our simple model has been implemented in the kinetic Monte Carlo code in order to investigate the boron diffusion, as shown in figure 1 [3]. In the KMC, a physical system, which consists of many possible events evolves as a series of independent events occurring. All events have their own event rates. Event rates are calculated from equation (1) wherein E_b is either migration-energy barriers for jump event or binding energies for clusters.

Further, v_0 is an attempt frequency, which is simply the vibrational frequency of the atom. In most cases, it is of

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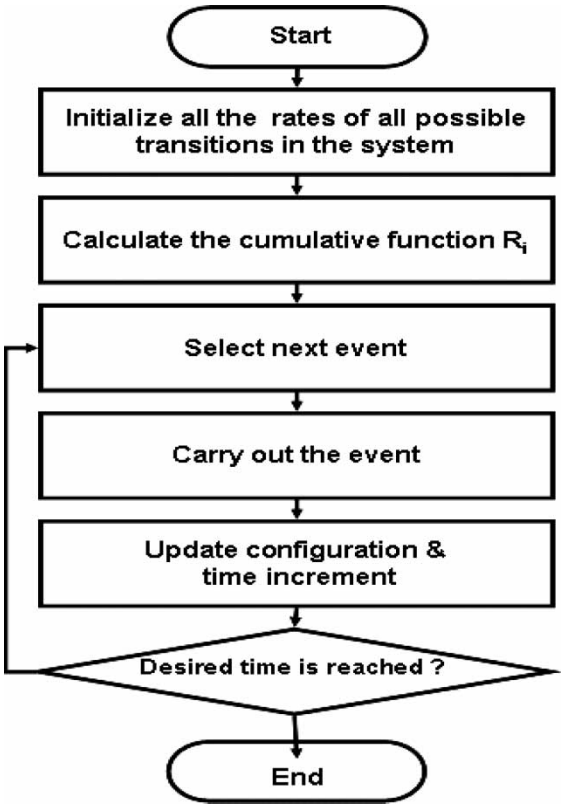

Figure 1. Kinetic-Monte Carlo algorithm.

the order of 1/1000 fs. Theses parameters are taken either from *ab initio* calculations or from experimental data.

$$v = v_0 \cdot E^{\left(\frac{-E_b}{K_B T}\right)} \tag{1}$$

Here, K_b and T represent Boltzmann's constant and absolute temperature, respectively. Now, let us consider thermally activated events in the thermal annealing process after ion implantation. If the probability for a subsequent event to occur is independent of the previous history and is not changing at all times, the transition probability is constant, which is so called a Poisson process. To derive the time dependence, consider a single event with a uniform transition probability r [4]. 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. This is because f gives the probability density wherein the physical system still remains at time t,

$$\mathrm{d}f(t) = -rf(t)\mathrm{d}t \tag{2}$$

Further, the solution is given by with boundary conditions,

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

Therefore, the simulation time is updated $t = t + \Delta t$ according to event rates as the following due to ensemble properties of independent *Poisson process*:

$$\Delta t = -\frac{\ln u}{R} \tag{4}$$

Here, u is a random number between 0 and 1 and R is the total sum of all possible event rates. Therefore, Δt, which is domain of time, increases as reducing R through events such as recombination, reaction, and sinking in the diffusion process. KMC is suitable for simulating non-uniform time evolution processes.

3. Simple atomistic model

The continuum models for B_mI_n clusters in boron diffusion have been widely investigated [3,13,15,17,19]. A large number of clusters are shown by solid circles in figure 2. The clusters were associated with a set of continuity equations and parameters. Recently, a research group led by Dunham in the University of Washington [1] suggested a simple continuum model for medium and low energy boron implants. Based on the analysis of cluster kinetics, the simple model was derived from the multi-cluster model. They reduced the number of cluster continuity equations from ten to just two involving the clusters, BI_2 and B_3I.

The simple atomistic model employs the interstitialcy mechanism wherein, impurities are supposed to diffuse in a mobile form of defect, which is denoted as BI (boron + interstitial pair). Generally, an interstitial tends to take its position where the energy is minimized, which means a stable site in silicon crystal structure. It has been found that tetrahedral site and hexagonal site are stable sites. During the annealing process, excited interstitials positioned at the interstitial site migrate through the above-mentioned interstitial sites. If an interstitial happens to react with boron in the lattice site, the interstitial and boron pair (BI) is formed and migrated from point to point. It was called the interstitialcy mechanism [9]. Thereafter, extended defects are formed from individual defects by encounter. The extended defects play a role in boron diffusion. We find that the simple atomistic model including only clusters BI_2 and B_3I is not quite enough to fit the SIMS data. As shown in figure 3, we now propose a model wherein BI_2 evolves to B_2I_3 or BI and B_2I_2 evolves to B_2I or B_3I_3. Namely, KMC simulations revealed that

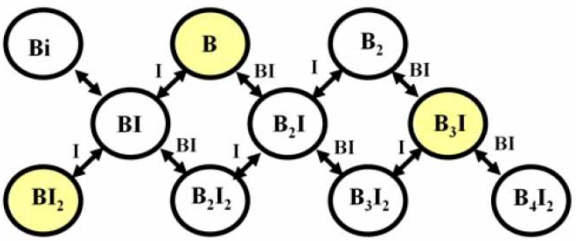

Figure 2. Clusters in full continuum model (solid line) and simple continuum model (shown in grey here, yellow in online version).

both B_2I_3 and B_3I_3 play a crucial role in the evolution of dominant clusters [16,18].

$$B_s + I \Leftrightarrow B_i \tag{5}$$

$$B_mI_n + I \Leftrightarrow B_mI_{n+1} \tag{6}$$

$$B_mI_n + B_i \Leftrightarrow B_{m+1}I_{m+1} \tag{7}$$

In our simple atomistic model, other clusters such as B_2I_3 and B_3I_3 were implemented. The evolution of clusters is modeled in equations (5) and (6).

4. Boron retardation

Since arsenic and boron atoms are crucial for CMOS process, the accurate model of those impurities is needed. Especially, the formation of ultra-shallow junction in nano-CMOS technology confronts several obstacles such as transient enhanced diffusion (TED), boron enhanced diffusion (BED) and oxide enhanced diffusion (OED). Consequently, investigations on ultra-low-energy ion implantation, rapid thermal annealing (RTA), co-implantation of boron and fluorine and boron retardation by arsenic pre-doped wafer experiences rapid progress in suppressing the anomalous diffusion.

We applied the boron retardation to arsenic pre-doped wafer in order to verify our simple atomistic model. After implantation, arsenic atoms migrate via reactions with interstitials and vacancies. It is believed that AsV and AsI, formed after reactions, are mobile while substitutional As is immobile in silicon. Further, arsenic evolves into clusters comprising arsenic and vacancy.

$$As_s + V \Leftrightarrow AsV \tag{8}$$

$$As_s + I \Leftrightarrow AsI \tag{9}$$

$$As_mV_n + V \Leftrightarrow As_mV_{n+1} \tag{10}$$

$$As_mV_n + I \Leftrightarrow As_mV_{n-1} \tag{11}$$

$$As_mV_n \Leftrightarrow As_mV_{n-1} + V \tag{12}$$

$$As_mV_n \Leftrightarrow As_mV_{n-1} + AsV \tag{13}$$

It turned out that AsV, AsI and As_mV_n clusters seem to play a role in arsenic diffusion. Mobile characteristics of arsenic atoms, however, seem to be worse than boron due to weight and volume. The migration and cluster binding energies are obtained from *ab initio* calculations, which analyze structure of electrons in atomic level [14]. Also, boron migrates via interstitial mechanism and evolves into cluster defects comprising interstitial, vacancy and interstitial boron.

$$B_s + I \Leftrightarrow BI \tag{14}$$

$$B_mI_n + I \Leftrightarrow B_mI_{n+1} \tag{15}$$

$$B_mI_n + V \Leftrightarrow B_mI_{n-1} \tag{16}$$

$$B_mI_n \Leftrightarrow B_mI_{n-1} + I \tag{17}$$

$$B_mI_n \Leftrightarrow B_{m-1}I_{n-1} + BI \tag{18}$$

Our KMC simulations revealed that boron competes with arsenic for reactions with interstitials, which leads to a conclusion that the retardation of boron occurs is more pronounced with donors than the case without donors.

5. Simulation results and discussion

5.1 Atomistic simple model

Now we are looking at the simple model. We constructed the basic structure of continuum model using dominant B, BI_2, and B_3I. Then, in order to utilize the cluster structure of simple continuum model, we created intermediate clusters acting as a bridge between dominant clusters. During our previous tests, the initial cluster structure induced more diffusion than we anticipated. So, in order to prevent such excessive diffusion, we also added two additional intermediate clusters in figure 3. Figure 3(b) is a schematic diagram illustrating dominant clusters and intermediate clusters in our simple atomistic model. Intermediate clusters impacting the evolution of dominant clusters are small in number as shown in figure 4.

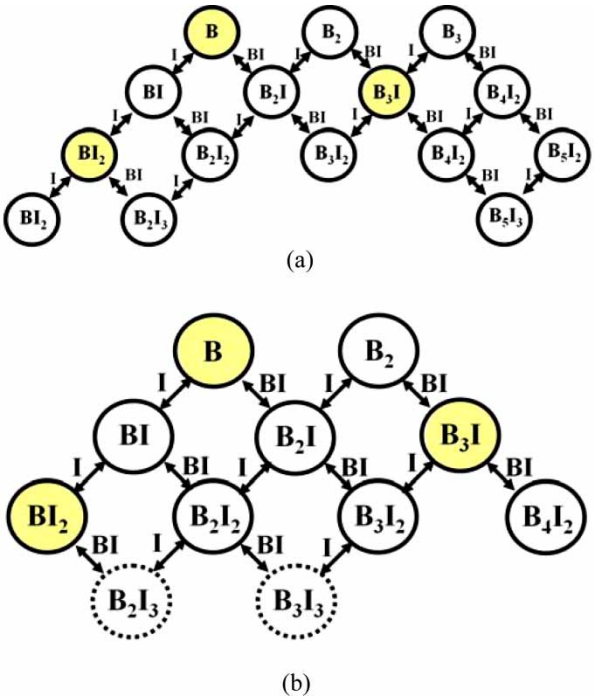

Figure 3. Clusters in (a) full atomistic model and (b) simple atomistic model and intermediate clusters (dotted line) in simple model.

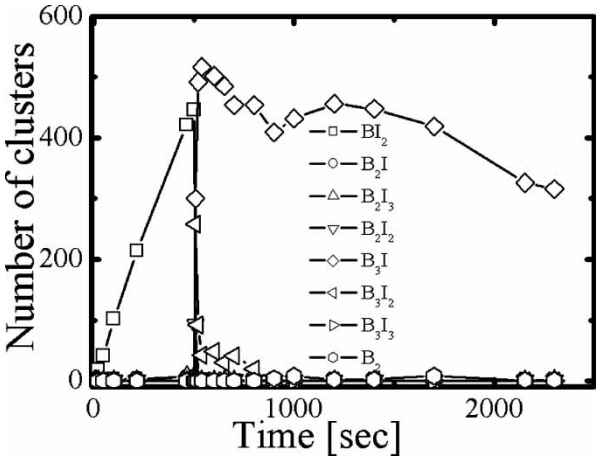

Figure 4. Number of clusters versus time for $5 \times 10^{14}\,cm^{-3}$, 20 keV boron implant, after 30 min anneal at 800°C.

However, those clusters play a role in the evolution of clusters. It should be noted that lifetimes of the intermediate clusters are short due to low binding energies. Figure 4 demonstrates the number of dominant clusters formed during the thermal annealing. In implantation and initial annealing, due to the fact that the event rate of interstitial is high, BI is created first of all, 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. The figure indicates boron interstitial clusters in accordance to time spent on annealing process. BI_2 clusters increased at the beginning of annealing process while B_3I increased suddenly at a later time period. Therefore, we were able to conclude that BI_2 and B_3I are the most dominant clusters. We discovered that the short-lived intermediate clusters not shown clearly in this figure play an important role. If we conducted this simulation without B_2I_3 and B_3I_3 in cluster structure, the number of B_3I clusters would have reduced significantly; such wasted interstitial would have created BI causing boron diffusion.

In figures 5 and 12, parameters of simple atomistic model are taken either from theoretical or from experimental total binding energies, which are needed to break up clusters and to migrate separated mobile defects. Figure 6 shows simulation results that extend defects like {311}, dislocation loops, B_mI_n clusters, etc. during annealing.

Figure 7 shows the boron profile for different ion implantation and annealing conditions; (a) $5 \times 10^{14}\,cm^{-2}$, 20 keV, followed by annealing at 800°C for 30 min, (b) $5 \times 10^{14}\,cm^{-2}$, 20 keV, followed by annealing at 800°C for 2 h, (c) $5 \times 10^{14}\,cm^{-2}$, 20 keV, followed by annealing at 900°C for 30 s, and (d) $2 \times 10^{14}\,cm^{-2}$, 20 keV, followed by annealing at 800°C for 1 h for the simple atomistic and the simple continuum models. These simulation results were performed based upon the above-mentioned conditions. In figure 7(a), the triangles (△) depict as-implantation SIMS profile, whilst the squares (□) represent SIMS profile after annealing. The upside down triangles (∇) indicate as-implantation using binary collision approximation (BCA), while the circles (○) show the annealing profile after changing the simple continuum profile to the simple atomistic profile. Finally, the diamonds (◇) represent the profile which we applied the simple atomistic model to through annealing process after changing the simple continuum model's atomistic clusters and adding B_2I_2 and B_3I_2 clusters. Consequently, we observed that the use of B_2I_2 and B_3I_2 enhanced the accuracy of the simulations.

Here is another simulation result under a different condition. Like the figure 7(a), we can obviously tell the difference between the circles (○) and the diamonds (◇) depending on the inclusion of B_2I_3 and B_3I_3. Thus, through the above simulation results, we, once again, confirmed the dominant cluster's characteristics resulted from changing simple continuum model to simple atomistic model and the importance of intermediate clusters acting as a bridge between clusters.

5.2 *Retardation of boron*

After co-implantation of B and As and performing annealing process, boron diffusion changes into a retardation condition,

AsV	1.01 (eV) (binding) 1.30(eV) (migration)	BI	0.1 (eV) (binding) 0.25 (eV) (migration)
As_2V	-3.5 (eV) (binding)	BI_2	-3.3 (eV) (binding)
As_3V	-4 (eV) (binding)	B_2I	-1.6 (eV) (binding)
As_4V	-5 (eV) (binding)	B_2I_2	-4.6 (eV) (binding)
AsI	0.1 (eV) (binding) 1.4 (eV) (migration)	B_2I_3	-6.0 (eV) (binding)
As_2	0 (eV) (binding)	B_3I	-3.6 (eV) (binding)
As_3	0 (eV) (binding)	B_3I_2	-6.0 (eV) (binding)
As_4	0 (eV) (binding)	B_3I_3	-6.0 (eV) (binding)
B_2	0.8 (eV) (binding)	B_4I_2	-6.5 (eV) (binding)

Figure 5. The binding and migration energies of arsenic, boron and As_mV_n, B_mI_n clusters. These energies are obtained from Theiss, *et al.* [5] and Cowern *et al.* [4].

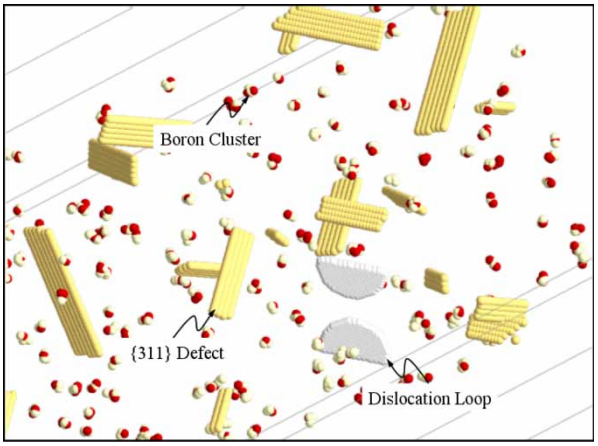

Figure 6. Extended defects: B_mI_n, {311}, dislocation loop.

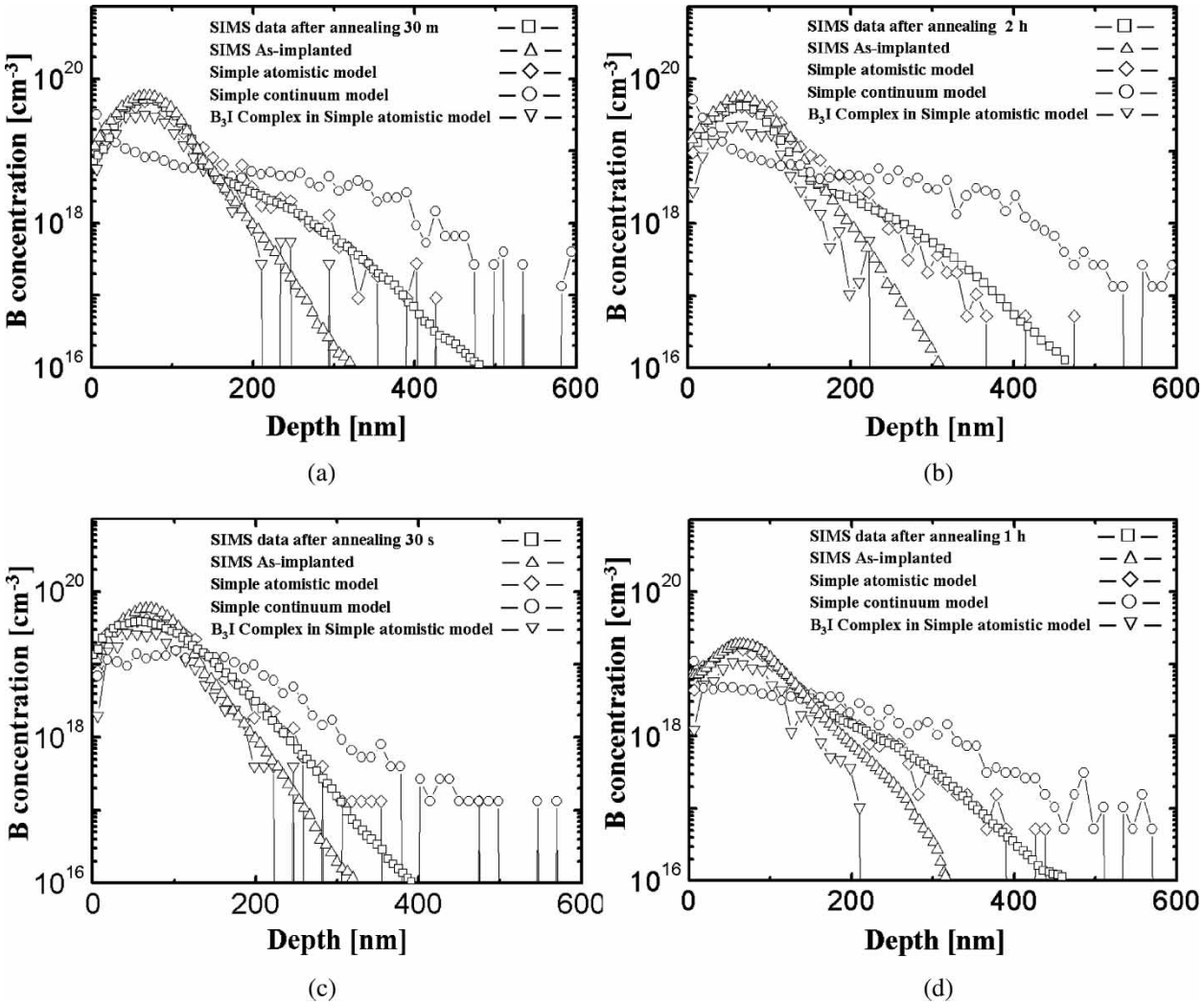

Figure 7. Comparison of simple atomistic model to SIMS and simple continuum model data for boron of $5 \times 10^{14}\,cm^{-2}$, 20 keV, (a), 800°C, for 30 min (b) 800°C, for 2 h (c) 900°C, for 30 s and (d) $2 \times 10^{14}\,cm^{-2}$, 800°C, for 1 h. SIMS is obtained from Giles *et al.* and Solmi *et al.* [6,7].

thus called boron retardation. Chakravathi *et al.* mentioned such theory as boron retardation [1,12]. He pointed out three factors that cause boron retardation; they are change of charge state due to co-implantation, effect on competitive binding of B and As to interstitial, and B and As paring effect.

However, we used B and As co-implantation of which we thought to be the most dominant mechanism out of the three boron retardation reasons. Our simple atomistic model showed results that are similar to SIMS data regarding the competitive effect between B and As. Thus, we concluded that the characteristics of B that uses interstitialcy mechanism and As that incorporates both interstitialcy mechanism and vacancy mechanism cause retardation of boron diffusion [10,11]. Of course, we need to apply the rest two boron retardation causes in order to achieve definitive results on even more microscopic testing environments.

In figure 8, the atomistic simulation results of boron with $5 \times 10^{14}\,cm^{-2}$, 20 keV, annealing for 4 h at 750°C and $5 \times 10^{14}\,cm^{-2}$, 20 keV, annealing for 20 min at 800°C in Si predoped with arsenic ($1.3 \times 10^{20}\,cm^{-3}$, low concentration (LC) and $6.0 \times 10^{19}\,cm^{-3}$, high concentration (HC)) and boron profile without pre-doped arsenic, are compared with SIMS data, respectively. It should be noted that the retardation of boron diffusion in silicon pre-doped with arsenic is more dominant than in the boron profile without arsenic. In figure 9, it shows the changes in interstitials when Boron of $1 \times 10^{14}\,cm^{-2}$, 10 keV, 800°C, for 20 min on Si wafer is pre-doped with As ($6.0 \times 10^{19}\,cm^{-3}$ (L.C.), $1.3 \times 10^{20}\,cm^{-3}$ (H.C.) and undoped. The time, 100 s, indicates the amount of interstitial at the rate of 1×10^{12} dose/s. Annealing begins after 100 s as shown on the figure. We can also clearly point out the change in interstitial as the wafer condition changes during the entire annealing process. We suggest that the interstitial binding resulted from dynamic annealing during implantation reduced the number of interstitials. After annealing begins, all interstitials drastically disappear at the beginning. Thus, As and interstitial binding happens very heavily as heating process prolongs. Therefore, such reaction reduces BI bonding resulting in boron retardation.

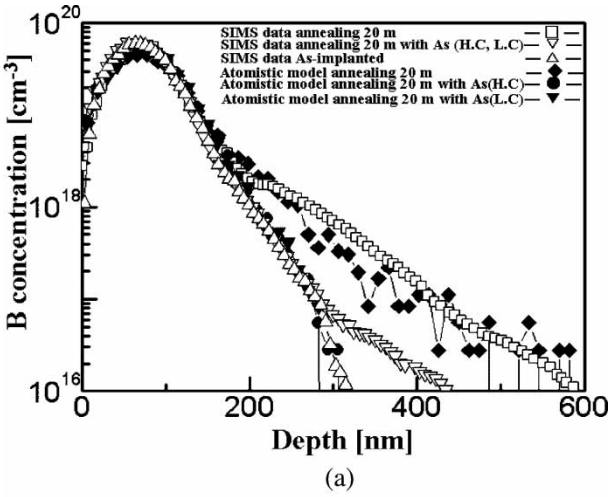

Figure 8. Comparison of simulation results of boron of $5 \times 10^{14}\,cm^{-2}$, 20 keV, 750°C, for 4 h and (b) $5 \times 10^{14}\,cm^{-2}$, 20 keV, 800°C, for 20 min in Si wafer predoped with As($6.0 \times 10^{19}\,cm^{-3}$(L.C.), $1.3 \times 10^{20}\,cm^{-3}$(H.C.) and undoped. SIMS is obtained from S. Solmi, *et al.* [6].

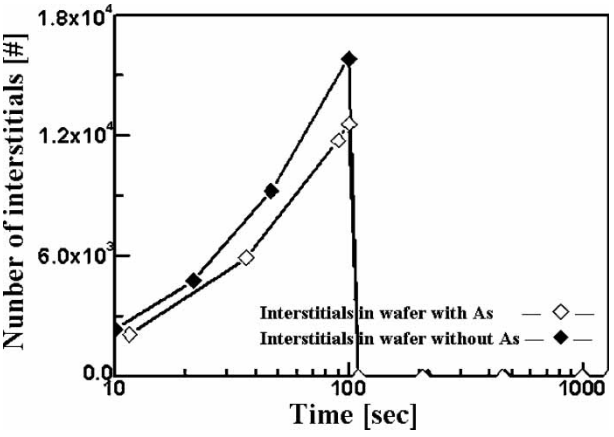

Figure 9. The time evolution of number of interstitials of boron of $1 \times 10^{14}cm^{-2}$, 10 keV, 800°C, for 20 min in Si wafer predoped with arsenic and Si wafer without arsenic.

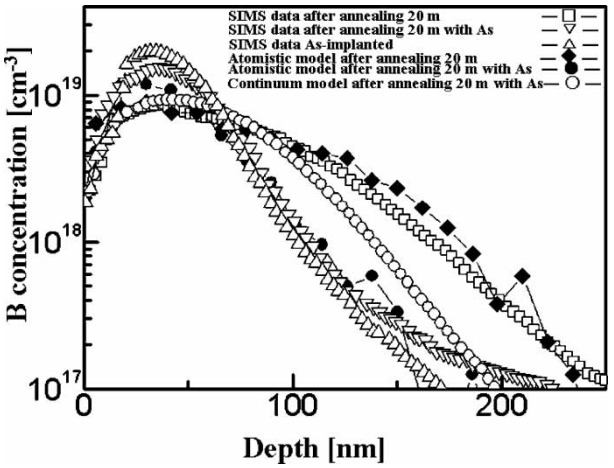

Figure 10. Comparison of simulation results of boron ($1 \times 10^{14}cm^{-2}$, 10 keV, 20 min annealing at 1000°C) in Si predoped with As ($6.0 \times 10^{19}\,cm^{-3}$ (LC), $1.3 \times 10^{20}\,cm^{-3}$ (HC), one undoped and Continuum model. SIMS is obtained from Solmi *et al*. [7].

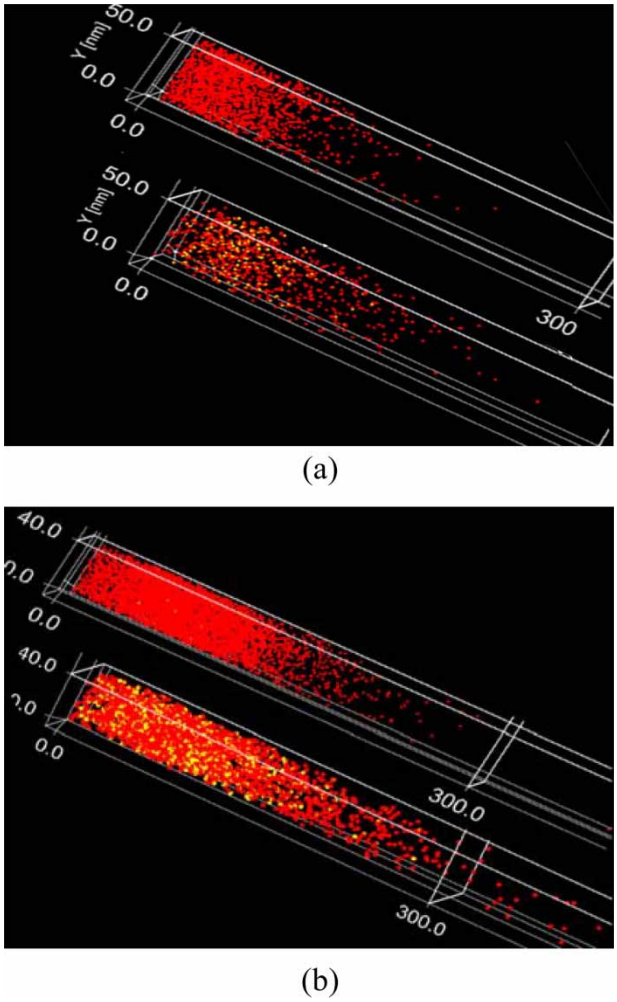

Figure 11. 3-D results of simulation results of boron of (a) $1 \times 10^{14}cm^{-2}$, (b) $5 \times 10^{14}cm^{-2}$, 10 keV, 800°C, for 20 min in Si wafer.

Experimental parameters [5]	Theoretical parameters [4]
Interstitial $D_i = 2$ cm^2/sec $E_m = 0.9$ eV	Interstitial $D_i = 5 \times 10^{-3}$ cm^2/sec $E_m = 1.0$ eV
Vacancy $D_v = 5 \times 10^{-6}$ cm^2/sec $E_m = 0.43$ eV	Vacancy $D_v = 1 \times 10^{-3}$ cm^2/sec $E_m = 0.4$ eV

Figure 12. Comparison of the parameters used in simple atomistic model.

Figure 10 shows the comparison of simulation results of boron with $1 \times 10^{14}\,\mathrm{cm}^{-2}$, 10 keV, 1000°C, 20 min annealing in SIMS, continuum model and atomistic model. In conclusion, our investigation reveals that boron is competitive with arsenic in reaction with interstitials for diffusion, which explains the retardation phenomenon of boron in silicon wafers pre-doped with arsenic from this motivation.

Figure 11 shows the 3-D profiles of boron. We could virtually note the distribution of 3-D simulation results of retardation of boron. This figure depicts the three dimensional results of figures from figure 10. Looking at figure 11(a), the upper picture is showing the effect of boron retardation and the lower picture indicates the normal state. We could clearly see the reduction of boron diffusion.

5.3 Experimental or theoretical parameters for interstitial and vacancy?

The parameters are crucial to enhance the accuracy of simulation. It is usual either to employ the experimental data or to use *ab initio* calculation in order to get the parameters. However, there may exist some discrepancies between experimental parameters and theoretical *ab initio* ones for interstitial and vacancy, wherein it is difficult to figure out which is correct [2]. In this work, both *ab initio* calculations [4] and experimental data [5] were employed to determine the event rates and to decide which event will follow next. Either theoretical parameters from *ab intio* calculations or experimental data were used in our model. Our simulation revealed that the accuracy of model seems to vary with scale of devices especially in nanometer regime.

Figure 12 shows the used parameters in the simple atomistic model. Figure 13 shows the comparison of simple atomistic model with theoretical or experimental parameters for boron of $5 \times 10^{14}\,\mathrm{cm}^{-2}$, 20 keV, (a), 800°C, for 30 min (b) 800°C, for 2 h. We applied the parameters to the simple atomistic model and found out that the theoretical parameters are more appropriate than the experimental data for our KMC simulations. We could observe the difference of results depending on theoretical or experimental parameters.

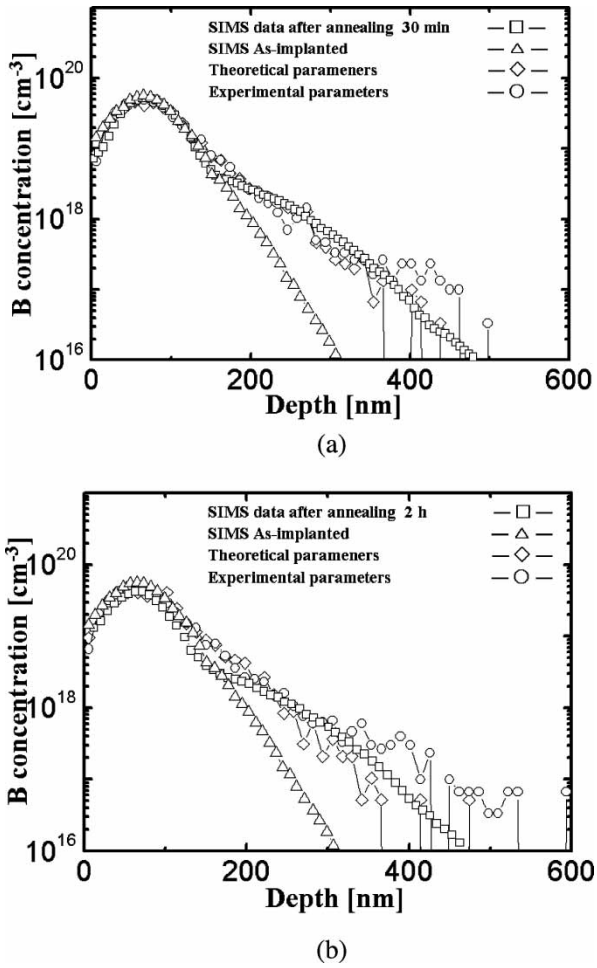

Figure 13. Comparison of simple atomistic model with theoretical or experimental parameters for boron of $5 \times 10^{14}\,\mathrm{cm}^{-2}$, 20 keV, (a), 800°C, for 30 min (b) 800°C, for 2 h. SIMS is obtained from Giles and Solmi *et al.* [6,7].

6. Conclusion

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

Also, we explained the role of donor in TED retardation of boron in silicon pre-doped with arsenic. Solmi *et al.* proposed three possible causes, which can result in boron TED retardation in silicon pre-doped with donor. In these atomistic simulations, only one of them can suffice to

explain the retardation. Boron and donor seem to compete with each other for reaction with interstitials atomistically.

We demonstrate that the theoretical parameters for interstitial and vacancy in the atomistic process are more appropriate than the parameters taken from the experimental data. The simple atomistic model implies that the depth profile in boron diffusion posterior to annealing with theoretical parameters is more accurate than the experimental ones with SIMS data. Finally, we implement these investigations based on the atomistic modeling approach; binary collision approximation (BCA) and kinetic Monte-Carlo (KMC) for ion implantation and diffusion, respectively.

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References

[1] S. Chakravathi, S.T. Dunham. A simple continuum model for boron clustering based on atomistic calculations. *J. Appl. Phys.*, **89**(7), 3650 (2001).
[2] B.W. Roberts, W. Luo, K.A. Johnson, P. Clancy. An order(N) tight-binding molecular dynamics study of intrinsic defect diffusion in silicon. *Chem. Eng. J.*, **74**, 67 (1999).
[3] M. Jaraiz, G.H. Gilmer, J.M. Poate, T.D. Rubia. Atomistic calculations of ion implantation in Si: Point defect and transient enhanced diffusion phenomena. *Appl. Phys. Lett.*, **68**(3), 409 (1996).
[4] S.K. Theiss, M.J. Caturla, T.J. Lenosky, B. Sadigh, T.D. Rubia, M.D. Giles, M.A. Foad. First-principles-based predictive simulations of B diffusion and activation in ion implanted Si, in IEDM Tech., Dig 18 (2000).
[5] N.E.B. Cowern, G. Mannino, P.A. Stolk, F. Roozeboom, H.G.A. Huizing, J.G.M. van Berkum, F. Cristiano, A. Claverie, M. Jaraiz. Energetics of self-interstitial clusters in Si. *Phys Rev Lett*, **82**(22), 4460 (1999).
[6] SIMS data from Intel Corporation.
[7] S. Solmi, F. Baruffaldi, R. Canteri. Diffusion of boron in silicon during post-implantation annealing. *J. Appl. Phys.*, **69**(4), 2135 (1991).
[8] K.A. Fichthorn, W.H. Weinberg. Theoretical foundations of dynamical Monte Carlo simulations. *J. Chem. Phys.*, **95**(2), 1090 (1991).
[9] S. Jihyun, K. Ohseob, K. Kidong, W. Taeyoung. Atomistic modeling and simulation of Boron diffusion in crystalline materials: KMC. *J. Korean Phys. Soc.*, **45**, S779 (2004).
[10] R. Pinacho, M. Jaraiz, P. Castrillo, J.E. Rubio, I.M. Bragado, J. Barbolla. Comprehensive, physically based modeling of As in Si. *Mat. Sci. Eng. B*, **114–115**, 135 (2004).
[11] L. Pelaz, G.H. Gilmer, V.C. Venezia, H.-J. Gossmann, M. Jaraiz, J. Barbolla. Modeling of the effects of dose rate, and implant temperature on transient enhanced diffusion. *Appl. Phys. Lett.*, **74**(140), 2017 (1999).
[12] S. Solmi, M. Bersani. Effects of donor concentration on transient enhanced diffusion of boron in silicon. *J. Appl. Phys.*, **87**(8), 3696 (1111).
[13] G.S. Hwang, W.A. Goddard. Diffusion of the diboron pair in silicon. *Phys. Rev. Lett.*, **89**(5), 055901 (2002).
[14] W. Windl, M.M. Bunea, R. Strumpf, S.T. Dunham, M.P. Masquelier. First-principles study of boron diffusion in silicon. *Phys. Rev. Lett.*, **83**(21), 4345 (1999).
[15] J.L. Blue, I. Beichl, F. Sullivan. Faster Monte Carlo simulations. *Phys. Rev. E*, **51**(2), R867 (1995).
[16] J. Yoo, C. Hwang, J. Seo, O. Kwon, T. Won. KMC simple model for B_mI_n cluster evolution during boron diffusion: Theoretical or experimental parameters of point defects. *NSTI Nanotech.*, **3**, 99 (2005).
[17] L. Shao, X. Lu, X. Wang, I. Rusakova, J. Liu, W. Chu. Retardation of Boron diffusion in Silicon by defect engineering. *Appl. Phys. Lett.*, **78**(16), 2321 (2001).
[18] J. Yoo, C.O. Hwang, J. Seo, O. Kwon, T. Won. Atomistic modeling for retardation of boron diffusion and dominant B_mI_n clusters in pre-doped silicon. *SISPAD*, (accepted) (2005).
[19] A.D. Lilak, S.K. Earles, K.S. Jones, M.E. Law, M.D. Giles. A Physics-based modeling approach for the simulation of anomalous boron diffusion and clusters behaviors. *IEDM Tech.*, 493 (1997).