Atomistic Modeling for Retardation of Boron Diffusion and Dominant B_mI_n Clusters in Pre-doped Silicon

Jae-Hyun Yoo, Chi-Ok Hwang, Byeong-Jun Kim and Taeyoung Won

Department of Electrical Engineering, School of Engineering, Inha University
253 Yonghyun-dong, Nam-gu, Incheon, Korea 402-751
Phone: +82-32-875-7436, Fax: +82-032-862-1350, E-mail: {twon, yjh}@hsel.inha.ac.kr

***Abstract* – In this paper, we present a simple atomistic model for describing the kinetic Monte Carlo (KMC) evolution of interstitial clusters during boron diffusion. It has been known that clusters generated after ion implantation play a decisive role in the enhanced boron diffusion at the tail region in contrast to the immobile property 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 understanding the evolutionary behavior of interstitial clusters during boron diffusion. We found out that the intermediate clusters such as B_3I_3 and B_2I_3 play a significant role despite that the lifetime of the corresponding intermediate clusters are relatively short due to low binding energies. Further, our investigation revealed that B_3I is the most dominantly acting cluster after annealing. We applied our simple atomistic model to the study of boron retardation in arsenic and phosphorous pre-doped substrate. Finally, KMC simulation results were compared with experimental data, which demonstrated an excellent agreement.**

I. INTRODUCTION

In order to model the diffusion process of impurities in silicon crystal, continuum models have been widely employed up to 100 nanometer process. Those employ 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 reaches nanometer regime. We propose an 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, 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, we investigated the boron retardation. Boron retardation is known as a phenomenon wherein boron diffusion via interstitial mechanism competes with arsenic and phosphorous diffusion via interstitial and vacancy mechanism in arsenic and phosphorous doped substrate.

II. DOMINANT B_mI_n CLUSTERS

The continuum models for B_mI_n clusters in boron diffusion have been widely investigated [2,3]. A large number of clusters are shown by solid circles in Fig. 1. The clusters were associated with a set of continuity equations and parameters. Recently, a research group led by S. T. Dunham in the University of Washington [2] suggested a simple continuum model for medium and low energy boron implants and thermal annealing. 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.

$$Bs + I \Leftrightarrow BsI \tag{1}$$

$$Bs_m I_n + I \Leftrightarrow Bs_m I_{n+1} \tag{2}$$

$$Bs_m I_n + BI \Leftrightarrow Bs_{m+1} I_{n+1} \tag{3}$$

$$Bs_m I_n + V \Leftrightarrow Bs_m I_{n-1} \tag{4}$$

$$Bs_m I_n \Leftrightarrow Bs_m I_{n-1} + I \tag{5}$$

$$Bs_m I_n \Leftrightarrow Bs_{m-1} I_{n-1} + BsI \tag{6}$$

The simple atomistic model employs the interstitialcy mechanism wherein impurities diffuse in the form of the mobile defect, BI. Thereafter, extended defects are formed from individual defects by encountering. 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 fig. 2, 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. In conclusion, KMC simulation revealed that both B_2I_3 and B_3I_3 play a crucial role in the evolution of dominant clusters. 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 Eqs. (2), (3) and (4).

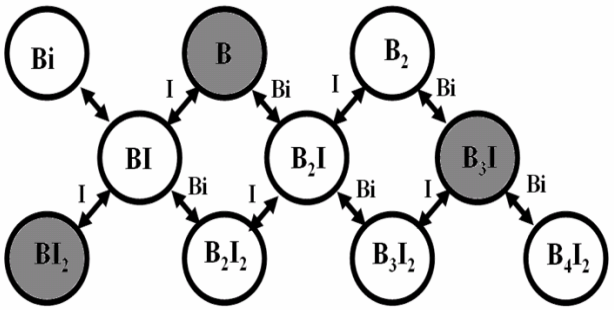
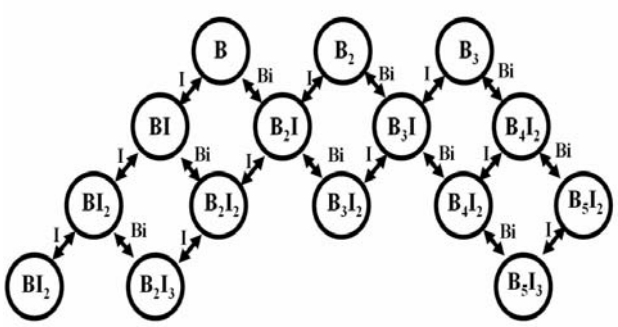
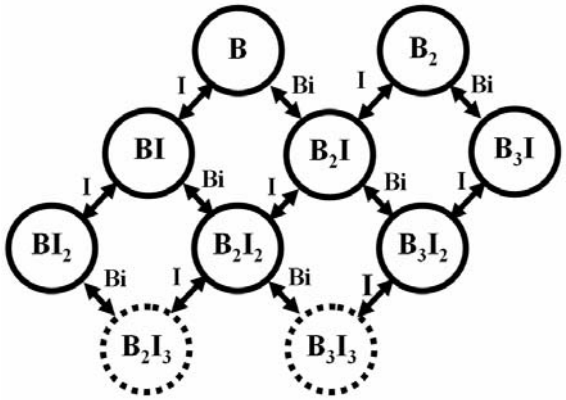


Figure 1: Clusters in full continuum model (solid lines) and simple continuum model (gray).



(a)



(b)

Figure 2: Clusters in (a) full atomistic model and (b) simple atomistic model and intermediate clusters (dotted line) in the simple model.

III. RETARDATION OF BORON

Since arsenic and boron atoms are crucial for CMOS process, the accurate model of those impurities is essential. Especially, the formation of ultra-shallow junction in nano-CMOS technology confronts several obstacles such as transient enhanced diffusion, boron enhanced diffusion and oxide enhanced diffusion. Consequently, investigations on ultra-low-energy ion implantation, rapid thermal annealing, co-implantation of boron and fluorine and boron retardation by donor pre-doped wafer experience rapid progress in suppressing the anomalous diffusion. We applied the boron retardation to donor pre-doped wafer in order to verify our simple atomistic model. After implantation of arsenic or phosphorus, arsenic or phosphorus migrates via reactions with interstitial and vacancy. We consider that AsV, AsI, PV and PI formed after reactions are mobile and substitutional As and P are immobile in Si. Also arsenic and phosphorus evolve into clusters composed of arsenic and vacancy or phosphorus and vacancy. The migration and cluster binding energies are obtained from *ab-initio* calculations [5]-[7].

$$As_s + V \Leftrightarrow AsV \quad (6)$$

$$As_s + I \Leftrightarrow AI \quad (7)$$

$$As_m V_n + V \Leftrightarrow As_m V_{n+1} \quad (8)$$

$$As_m V_n + I \Leftrightarrow As_m V_{n-1} \quad (9)$$

$$As_m V_n + AsV \Leftrightarrow As_{m+1} V_{n+1} \quad (10)$$

$$As_m V_n + AsI \Leftrightarrow As_{m+1} V_{n-1} \quad (11)$$

$$As_m V_n \Leftrightarrow As_m V_{n-1} + V \quad (12)$$

$$As_m V_n \Leftrightarrow As_{m-1} V_{n-1} + AsV \quad (13)$$

or

$$P_s + V \Leftrightarrow PV \quad (14)$$

$$P_s + I \Leftrightarrow PI \quad (15)$$

$$P_m V_n + V \Leftrightarrow P_m V_{n+1} \quad (16)$$

$$P_m V_n + I \Leftrightarrow P_m V_{n-1} \quad (17)$$

$$P_m V_n + PV \Leftrightarrow P_{m+1} V_{n+1} \quad (18)$$

$$P_m V_n + PI \Leftrightarrow P_{m+1} V_{n-1} \quad (19)$$

$$P_m V_n \Leftrightarrow P_m V_{n-1} + V \quad (20)$$

$$P_m V_n \Leftrightarrow P_{m-1} V_{n-1} + PV \quad (21)$$

It turns out that mobile donor and donor clusters seem to play a role in diffusion of donor. Mobile characteristics of donor atoms, however, seem to be worse than boron due to weight and volume. Our KMC simulations revealed that boron competes with donor for reactions with interstitials, which leads to the conclusion that the retardation of boron is more pronounced with donors than the without donors.

IV. SIMULATION RESULTS & DISCUSSION

In Figs. 3 and 4, the atomistic simulation results of boron with 10 keV, 1 x 10^{14} cm^{-2} and 20 keV, 5 x 10^{14} cm^{-2}, 20 min annealing at 800 ℃ in Si pre-doped with arsenic (1.3 x 10^{20} cm^{-3}, low concentration (LC) and 6.0 x 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. Figure 5 shows the boron profiles with 5 x 10^{14} cm^{-2}, 20 keV, 4 h annealing at 750 ℃. Figure 6 shows the comparison of atomistic simulation results of boron with 10 keV, 1 x 10^{14} cm^{-2} and 20 min annealing at 1000 ℃ with SIMS and continuum model. Figures 7 and 8 show the 3-D profiles of boron. We could virtually note the distribution of 3-D simulation results of retardation of boron diffusion. Figure 9 shows the atomistic simulation results of boron with 20 keV, 5 x 10^{14} cm^{-2}, 20 min annealing at 800 ℃ in Si predoped with phosphorous (1.2 x 10^{20} cm^{-3}, low concentration (LC) and boron profile without predoped phosphorous, are compared with SIMS data.

In Fig. 10, the time evolution of the number of interstitials is shown. The number of interstitials almost reduces in early annealing abruptly. We could clearly note the difference of interstitial reductions between in Si pre-doped with arsenic or phosphorus and one without pre-doped arsenic or phosphorus. Competition of boron and arsenic or phosphorus for reaction with interstitials causes the difference in the interstitial reduction. In Figs. 11 and 12, the dominant B_mI_n clusters in the atomistic model and the time evolution of the number of clusters is shown. Figure 13 shows the comparison of the atomistic simulation results of boron with 20 keV, 5 x 10^{14} cm^{-2} and 10 keV, 1 x 10^{14} cm^{-2}, 20 min annealing at 800 ℃ in Si pre-doped with Phosphorus (1.2 x 10^{20} cm^{-3} (HC)) model and boron profile without pre-doped arsenic with SIMS. We implement the boron diffusion with simple atomistic model concerning dominant B_mI_n clusters model.

CONCLUSION

In this paper, we presented an atomistic explanation for the role of donors in boron TED-related retardation in silicon which is pre-doped with arsenic or phosphorus. We found out that the intermediate clusters such as B_3I_3 and B_2I_3 play a significant role despite that the lifetime of the corresponding intermediate clusters are relatively short due to low binding energies. We applied our simple atomistic model to the study of boron retardation in arsenic and phosphorous pre-doped substrate. Boron and donor seem to compete with each other for reaction with interstitials. Also, we investigate the role of clusters in the atomistic process by comparing it with SIMS data and simple atomistic model results. We confirm that B_3I is the most dominant cluster in boron diffusion after annealing. We find that intermediate clusters play an important role in atomistic model and that distribution of boron in process can be simulated with the simple atomistic model.

ACKNOWLEGEMENTS

This work was supported partly by the Korean Ministry of Information & Communication (MIC) through the Information Technology Research Center (ITRC) Program supervised by IITA, and partly by the Korean Ministry of Science and Technology (MOST) through TND program and the international cooperative research program by KISTEP.

REFERENCES

[1] Jihyun Seo, *et al.*, J. Korean Phys. Soc, **45**, p. S779 (2004).
[2] S. Kravathi, and S. T. Dunham, J. Appl. Phys. **89**(7), p. 3650 (2001).
[3] Loudes Pelaz., Appl. Phys. Lett., **74**, p. 3657 (1999).
[4] S. Solmi, *et al.*, J. Appl. Phys., **87**, p. 3696 (2000).
[5] S. K. Theiss, *et al.*, Thin Solid Films., p. 219 (2000)
[6] N. E. B. Cowern, *et al.*, Phys. Rev. Lett., **82**, p. 409 (1999).
[7] R. Pinacho, *et al.*, Materials Science and Engineering B 114-115., p. 135 (2004).
[8] S. Solmi, *et al*, Journal of Applied physics, **69**, p. 2135 (1991).
[9] J. Yoo, *et al.*, NSTI Nanotech **3**, p. 99 (2005).
[10] A. D. Lilak, *et al.*, in IEDM Tech., p. 493 (1997).
[11] L. Shao, *et al.*, Appl. Phys. Lett., **78**(16), p. 2321 (2001).
[12] K. Fichthorn, *et al.*, J. Chem. Phys. **95**(2), p. 1090 (1991).

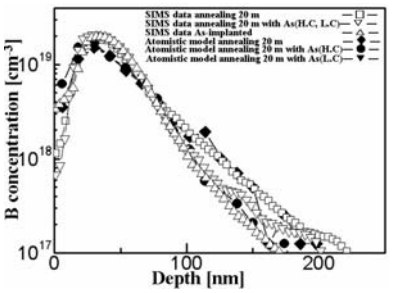


Figure 3: Comparison of simulation results of boron of 1 x 10^{14} cm^{-2}, 10 keV, 800 ℃, for 20 min in Si wafer predoped with As (6.0 x 10^{19} cm^{-3} (L.C.), 1.3 x 10^{20} cm^{-3} (H.C.) and undoped. SIMS is obtained from S. Slomi, *et al.*, [4].

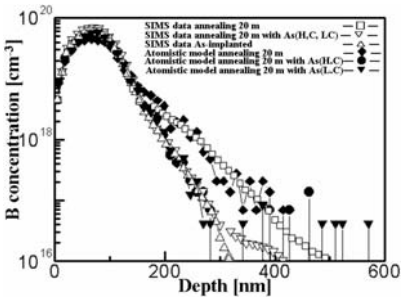


Figure 4: Comparison of simulation results of boron of 5 x 10^{14} cm^{-2}, 20 keV, 800 ℃, for 20 min in Si wafer predoped with As (6.0 x 10^{19} cm^{-3} (L.C.), 1.3 x 10^{20} cm^{-3} (H.C.) and undoped. SIMS is obtained from S. Slomi, *et al.*, [4].

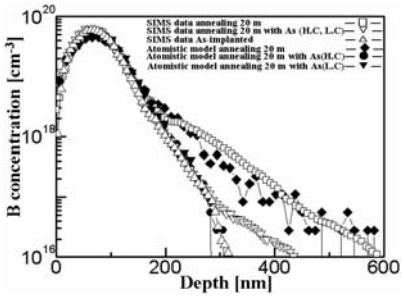


Figure 5: Comparison of simulation results of boron of 5 x 10^{14} cm^{-2}, 20 keV, 750 ℃, for 4 h in Si wafer predoped with As (6.0 x 10^{19} cm^{-3} (L.C.), 1.3 x 10^{20} cm^{-3} (H.C.) and undoped. SIMS is obtained from S. Slomi, *et al.*, [4].

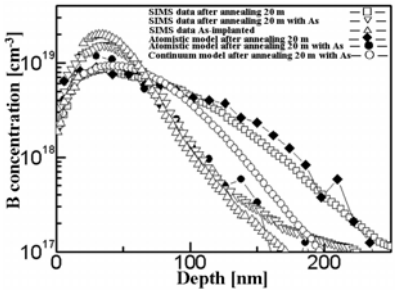


Figure 6: Comparison of simulation results of boron of 1 x 10^{14} cm^{-2}, 20 keV, 800 ℃, for 20 min in Si wafer predoped with As (6.0 x 10^{19} cm^{-3} (L.C.)), undoped with As and continuum simulation. SIMS is obtained from S. Slomi, *et al.*, [4].

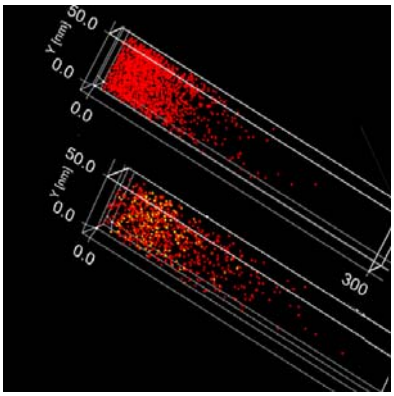


Figure 7: 3-D result of simulation results of boron of 1 x 10^{14} cm^{-2}, 10 keV, 800 ℃, for 20 min in Si wafer.

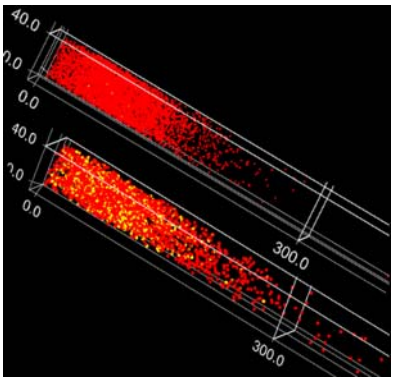


Figure 8: 3-D result of simulation results of boron of 5 x 10^{14} cm^{-2}, 20 keV, 800 ℃, for 20 min in Si wafer.

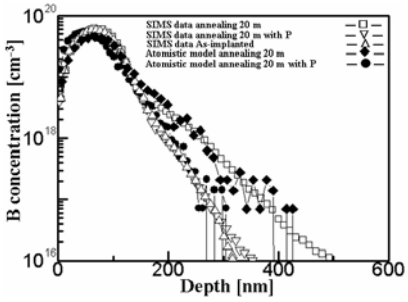


Figure 9: Comparison of simulation results of boron (20 keV, 5 x 10^{14} cm^{-2}, 20 min annealing at 800 ℃) in Si predoped with P (1.2 x 10^{20} cm^{-3}) and undoped. SIMS is obtained from S. Solmi, *et al.*, [4].

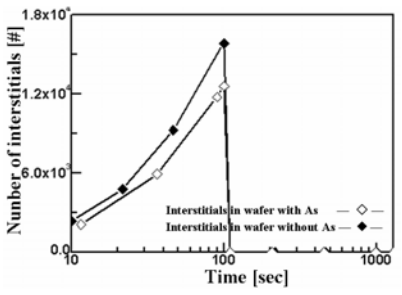


Figure 10: Time evolution of number of interstitials of boron of 1 x 10^{14} cm^{-2}, 10 keV, 800 ℃, for 20 min in Si wafer predoped with arsenic and Si wafer without arsenic.

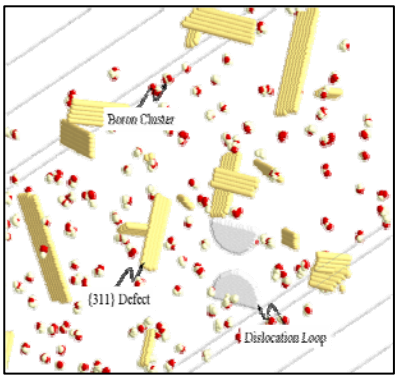


Figure 11: 3-D B_mI_n clusters and extended defects in boron diffusion.

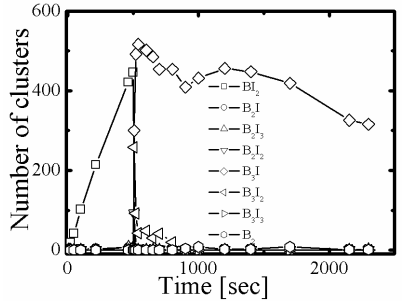
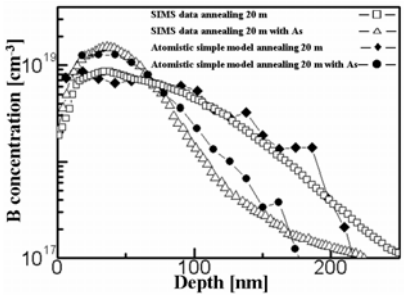
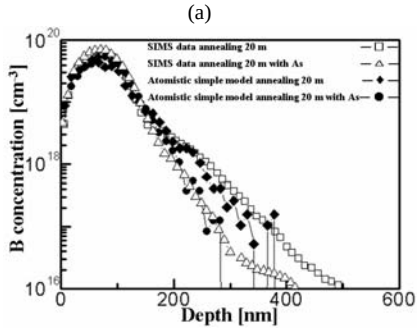


Figure 12: Number of clusters versus time for 30min anneal at 800 ℃ after 5 x 10^{14} cm^{-2}, 20keV boron implant.



(a)



(b)

Figure 13: Comparison of simulation results of boron of (a) 1 x 10^{14} cm^{-2}, 20 keV, (b) 5 x 10^{14} cm^{-2}, 20 keV, 800 ℃, for 20 min in Si wafer predoped with As(1.3 x 10^{20} cm^{-3} (H.C.)), undoped with As and atomistic simple model.