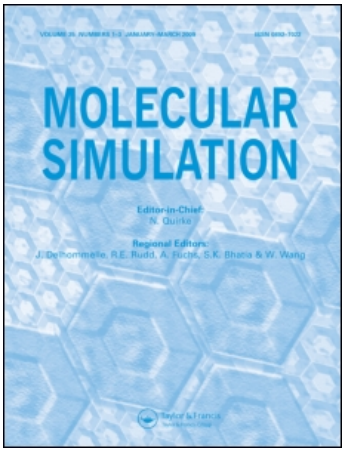

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Minimised atomistic model and main evolution path for dominant B_mI_n clusters in boron diffusion

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In this paper, we report our study on the minimised atomistic model (MAM) and the determination of an evolution path for dominant B_mI_n clusters during boron diffusion in kinetic Monte Carlo (KMC). 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 MAM, based on the simple continuum model and the simple atomistic model, takes the smallest number of intermediate clusters into account as well as dominant clusters for the evolution path of interstitial clusters during boron diffusion. We find that intermediate clusters such as B_2I_3 and B_3I_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. Also, through our simulation results, we find the main evolution path of dominant clusters from B_2I to B_3I during thermal annealing in the MAM. Furthermore, our investigation reveals that the density of BI_2 clusters increases at the beginning of the annealing process while the density of B_3I increases at a later stage. KMC simulation results are compared with experimental SIMS data, which support our theoretical model.

Keywords: minimised atomistic model; B_mI_n clusters; boron diffusion; kinetic Monte Carlo

1. Introduction

As complementary metal-oxide semiconductor (CMOS) devices are scaled down into the nanometer regime, they become even more stringent to control the impurity profiles at the front-end process. In order to model the S/D junction of impurities in nano CMOS devices, continuum models have been widely employed for up to 100 nm processes, and employ deterministic methods such as finite difference methods or finite element methods. The continuum models are considered to be tolerably accurate for explaining the diffusion process in the submicron regime. However, the accuracy becomes poorer as the scale of devices reaches the nanometer regime. These days, as an alternative, process engineers use in devices atomistic models such as the kinetic Monte Carlo (KMC) method to get more accurate simulation results from boron diffusion [1–4]. The above-mentioned KMC is based on the Monte Carlo approach combined with the Poisson process. It was found that this method can calculate more accurately than continuum models due to simulation into the atomic level. However, the atomistic model has some problems simulating impurity diffusion. First of all, a number of parameters, like migration energies and binding energies of impurities and defects, are difficult to obtain and a lot of computing time is required for the parameter calculation. The atomistic model needs a lot of CPU time to simulate impurity diffusion. In particular, because boron has many complex clusters, it is the most difficult to model and implement.

In our previous work [5], we implemented an approximate work of boron clusters to resolve the problems observed in the atomistic model such as difficulty of embodiment and high consumption of CPU time. We proposed a simple atomistic model including dominant clusters and intermediate clusters in order to simplify the complicated boron diffusion processes in Figures 1 and 2. For the approximation, we investigated atomistic modelling using binary collision approximation [6,7] and the KMC method [8,9].

In this paper, we refine the previous work and present a minimised atomistic model (MAM) and an evolution path in boron diffusion. The MAM simulates the boron diffusion more efficiently. We also find the main evolution path from B_2I to B_3I. Therefore, we confirm that B_2I_3 and B_3I_3 play a crucial role in the formation of the main evolution path and that B_3I is the dominant cluster in boron diffusion.

2. Minimised atomistic model and evolution path of dominant clusters

Through the results of the previous work [5], we confirm that BI_2 and B_3I are the dominant clusters in our

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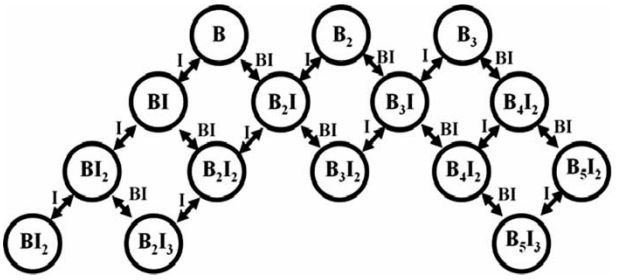

Figure 1. B_mI_n clusters structure in full atomistic model.

simple model. Additionally, we discover that short lived intermediate clusters like B_2I_3 and B_3I_3 play a crucial role. 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 minimised, which means stable sites in silicon crystal structure. It has been found that tetrahedral sites and hexagonal sites are stable sites. During the annealing process, excited interstitials positioned at the interstitial sites migrate through the above-mentioned interstitial sites. If an interstitial happens to react with boron in the lattice site, BI is formed and migrated. It is called the interstitialcy mechanism [10]. Thereafter, extended defects are formed from individual defects by encounter. The extended defects play a role in boron diffusion.

We refine the previous simple atomistic model and propose a MAM including dominant clusters and intermediate clusters. The MAM can be easily implemented in the atomistic approach. Through analysing our simulation results for the evolution of clusters versus time in Figure 4, we determine the dominant clusters and the importance of some intermediate clusters such as B_2I_3 and B_3I_3. So, in our MAM, we realise that B_2 and B_2I in our simple atomistic model are not that important to simulating boron diffusion. Consequently, we remove B_2 and B_2I in the simple atomistic model so that the MAM is able to simulate boron diffusion using as small as possible a number of the clusters as shown in Figure 3.

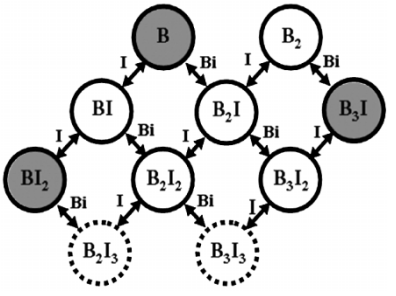

Figure 2. Simple continuum model (gray) [11] and our previous simple atomistic model [5].

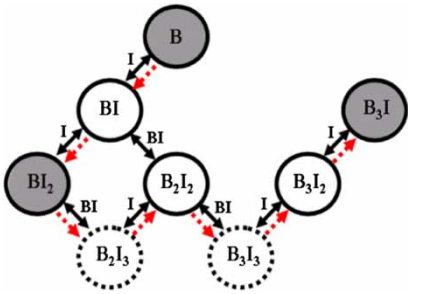

Figure 3. Minimised atomistic model (MAM) and the evolution path of dominant clusters (red dotted arrow).

The evolution of clusters is modelled in Equations (2.1)–(2.3). Through the main evolution path of dominant clusters in Figure 3 (red dotted arrow), we confirm that intermediate clusters play an important role in the evolution of clusters.

$$B_s + I \Leftrightarrow B_i \tag{2.1}$$

$$B_mI_n + I \Leftrightarrow B_mI_{n+1} \tag{2.2}$$

$$B_mI_n + B_i \Leftrightarrow B_{m+1}I_{m+1}. \tag{2.3}$$

3. Simulation results and discussion

In the previous work [5], we tried to implement a simple atomistic model constructed following the simple continuum model [11] using dominant B, BI_2, and B_3I. Then, during an effort to utilise the simple continuum model, we realised that we needed the intermediate clusters to act as a bridge between the dominant clusters in

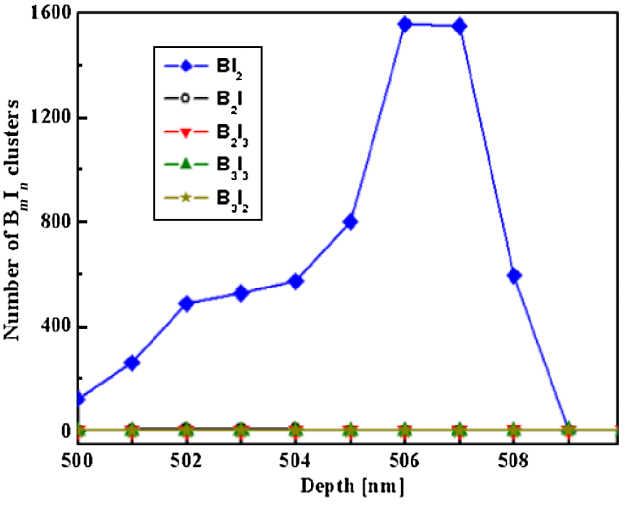

Figure 4. Number of clusters versus time for $5 \times 10^{14}\,cm^{-3}$, 20 keV boron implant, after a 30 min anneal at 800°C between 500 and 510 s in the first trial model without B_2I_3 and B_3I_3.

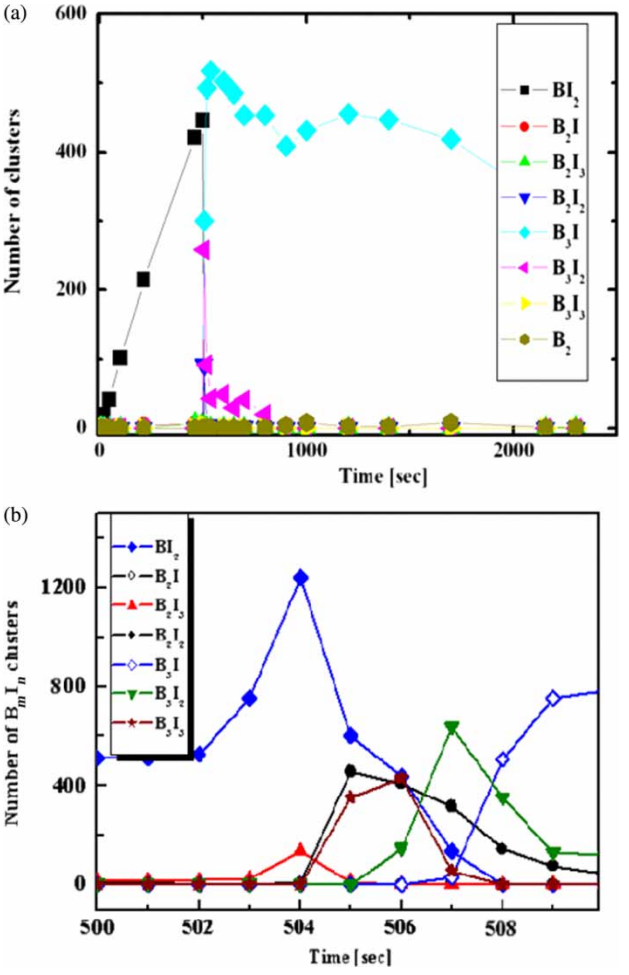

Figure 5. Number of clusters versus time for $5 \times 10^{14}\,cm^{-3}$, 20 keV boron implant, after a 30 min anneal at 800°C (a) in the simple atomistic model (b) between 500 and 510 s in the simple atomistic model.

the first trial model. When we conducted this simulation without B_2I_3 and B_3I_3, the B_3I clusters were not found (Figure 4); such lost interstitials would have created BI causing boron diffusion. Therefore, we were able to confirm the role of B_2I_3 and B_3I_3 in the evolution path of dominant clusters in boron diffusion during thermal annealing.

During our first trial model test, the initial simple atomistic model induced more diffusion than the full atomistic model (see Figure 1) [5]. So, in order to prevent such excessive diffusion, we added two further intermediate clusters. Figure 2 is a schematic representation illustrating the dominant clusters and intermediate clusters in our simple atomistic model. The intermediate clusters impacting the evolution of dominant clusters are small in number, as shown in Figure 5(a). However, those clusters play a role in the evolution of clusters. It should be noted that the lifetimes of the intermediate clusters are short due to low binding energies.

Time	BI_2	B_2I	B_2I_3	B_2I_2	B_3I	B_3I_2	B_3I_3	B_2
500	513	9	17	1	1	2	1	0
501	514	9	17	1	1	2	1	0
502	528	1	18	1	1	2	1	0
503	755	1	24	1	1	2	1	0
504	1240	1	135	9	1	2	2	0
505	603	1	12	456	1	1	353	0
506	437	1	0	407	1	148	431	0
507	134	1	0	317	28	638	56	0
508	1	1	1	144	508	352	1	0
509	1	1	1	78	753	132	1	0
510	1	1	1	47	781	118	1	0
511	1	1	1	27	783	120	1	0
512	1	1	1	23	772	132	1	0
513	1	1	1	0	781	118	1	0
514	1	1	1	0	782	102	1	0
520	1	1	1	2	492	92	1	0
540	1	1	1	4	517	43	1	0
600	1	1	1	1	502	49	1	0
650	1	1	1	2	485	30	1	0
700	1	1	1	1	454	41	1	0
800	1	1	1	1	454	20	1	0
900	1	1	1	1	409	1	1	0

Figure 6. From Figure 4(b), time evolution of number of clusters is shown.

Figure 5(a) demonstrates the number of dominant clusters formed during thermal annealing in the simple atomistic model [5]. In implantation and initial annealing, due to the fact that the event rate of interstitial migration is high, BI is created first of all, and then BI_2 becomes the dominant cluster while the other defects recombine and form the extended defects. However, B_3I becomes the

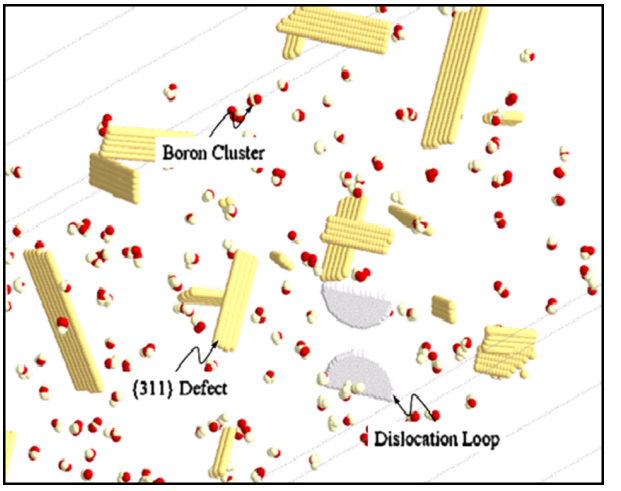

Figure 7. Extended defects: B_mI_n, {3 1 1}, dislocation loop.

most dominant cluster within a second. Therefore, we are able to conclude that BI_2 and B_3I are the most dominant clusters. Figure 5(b) depicts the boron-interstitial clusters between 500 and 510 s (see Figure 5(a)). As shown on the graph, we were able to determine the evolution path of the dominant clusters. We discovered that the short lived intermediate clusters form the evolution path of dominant clusters in boron diffusion in Figures 5(b) and 6. In Figures 5(b) and 6, we learn that the evolution of B_2 and B_2I in the simple atomistic model scarcely occurs. Therefore, we propose the MAM that has the simplest possible clusters (Figure 3).

In Figure 7, it is shown that we could observe extended defects like {3 1 1}, dislocation loops, B_mI_n clusters, etc. during annealing.

Figure 8 shows the boron profiles for different ion implantations 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, (d) $2 \times 10^{14}\,cm^{-2}$, 20 keV, followed by annealing at 800°C for 1 h for the MAM. These simulation results were performed based upon the above-mentioned conditions. In Figure 8(a), the green colour–dotted line depicts as-implantation SIMS profile, while the green colour–bold line represents SIMS profile after annealing. The blue colour–empty diamonds (◇) indicate as-implant profile using binary collision approximation, while the blue colour–filled diamonds (◆) represent the profile which we applied to our MAM through annealing process. Finally, the red upside down triangles (▼) indicate the profile of B_3I clusters after the annealing process. Consequently, we observe that the MAM excluding B_2 and B_2I in the simple atomistic model is able to simulate the boron diffusion and that B_3I plays a crucial role in boron diffusion. Figure 8(b)–(d) shows the other simulation results under different conditions. As in Figure 8(a), we can obviously tell the coincidence between the green

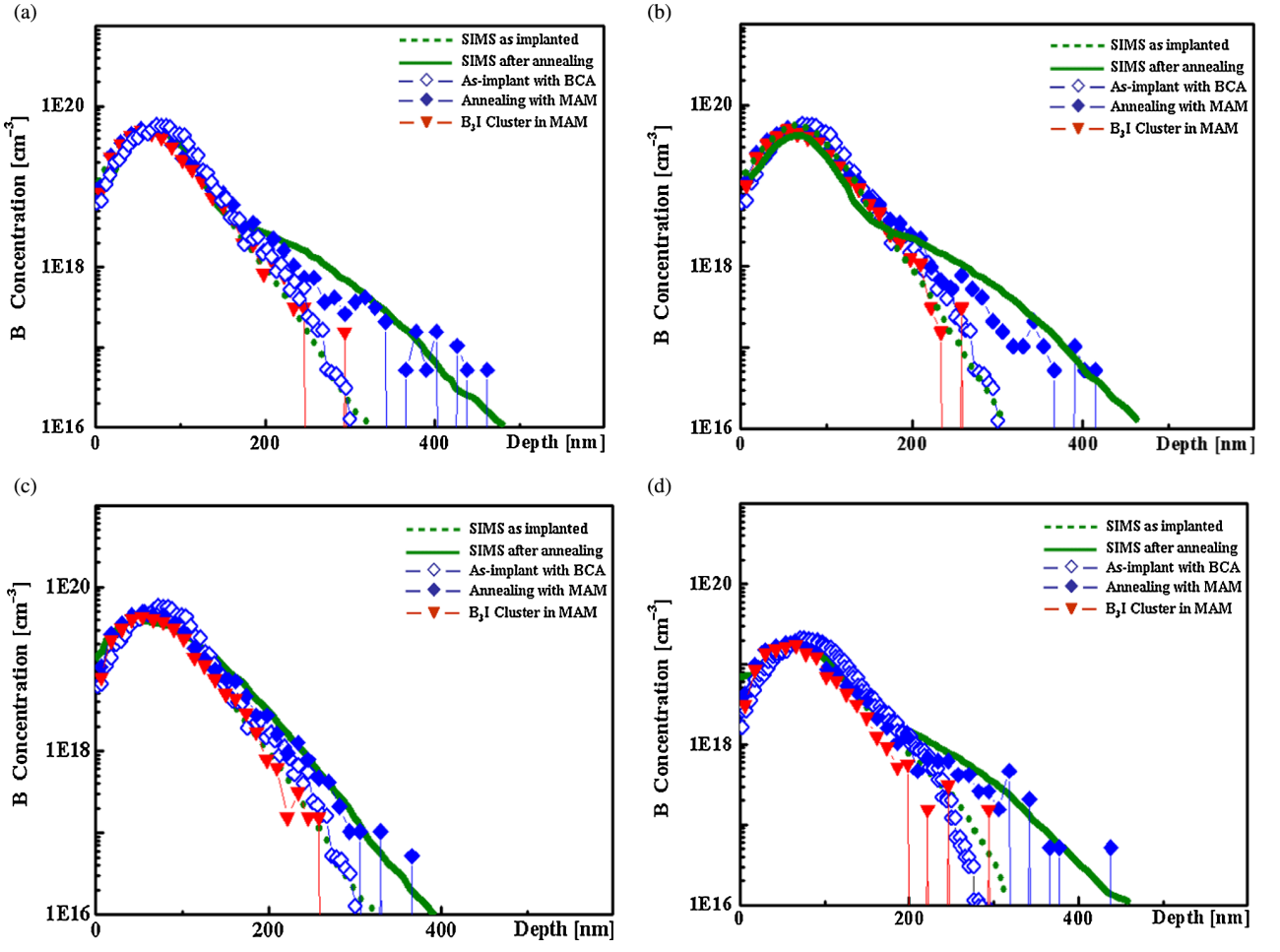

Figure 8. Boron profiles for different ion implantations and annealing conditions; (a) $5 \times 10^{14}\,cm^{-2}$, 20 keV, followed by annealing at 800°C for 30 min, (b) $5 \times 10^{14}\,cm^{-2}$, 20 keV, followed by annealing at 800° for 2 h, (c) $5 \times 10^{14}\,cm^{-2}$, 20 keV, followed by annealing at 900°C for 30 s, (d) $2 \times 10^{14}\,cm^{-2}$, 20 keV, followed by annealing at 800°C for 1 h for the MAM. SIMS is obtained from Giles et al., S. Solmi, et al. [10,12,13].

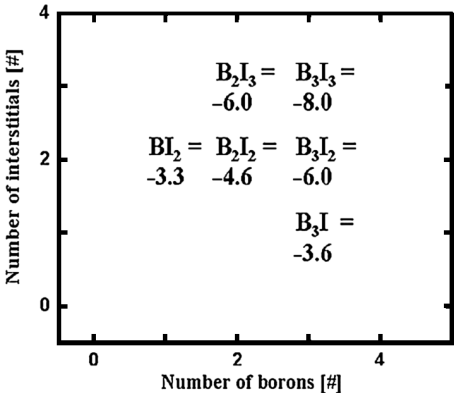

Figure 9. Binding energies of B_mI_n clusters. These energies are obtained from Theiss et al. [3] and Cowern et al. [9,10].

colour–bold lines and the blue colour–filled diamonds (◆). Thus, through the above simulation results, we once again confirm the importance of intermediate clusters acting as a bridge between clusters. Also, through our simulation results (Figure 8), we were able to determine that B_2I_3 and B_3I_3 play a crucial role in the evolution path of dominant clusters in boron diffusion due to the evolution path consisting of such intermediate clusters (see Figure 3). Figure 9 shows the binding energies of boron used in the MAM, which are needed to break up clusters and to migrate separated mobile defects [14,15].

4. Conclusions

In our previous work, we implemented a simple atomistic model [5] to simplify the complex boron-interstitial clusters based on B, BI_2, and B_3I of simple continuum model [11] in boron diffusion process. We confirmed that the results of the simple atomistic model agree with SISM considerably. In this paper, we refine the simple atomistic model to MAM. In the results of our MAM, we find the evolution path of dominant clusters and the simplest possible cluster model to simulate boron diffusion. Through the simulation results, we exclude B_2, B_2I from the simple atomistic model. In our MAM, we also confirm that B_3I is the most significant cluster in the boron diffusion during thermal annealing like the simple atomistic model. We find out that the intermediate clusters like B_2I_3 and B_3I_3 should be taken into account for an accurate KMC simulation and that such intermediate clusters form the evolution path of dominant clusters.

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