

Atomistic Simulation of RTA Annealing for Shallow Junction Formation characterizing both BED and TED

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Abstract – An atomistic model for annealing simulation is presented. To well simulate both BED (Boron Enhanced Diffusion)^[1] and TED (Transient Enhanced Diffusion), the surface emission model, which describes the emission of point defects from surface during annealing, is implemented. The simulation is carried out for RTA annealing (1000 °C or 1050 °C) after B implantation. The implantation energy varies from 0.5keV to 13keV. Agreements between simulation and SIMS data are achieved. Both BED and TED phenomena are characterized. The Enhancement of diffusion is discussed.

I. INTRODUCTION

Shallow junctions are needed in deep sub-micron devices to suppressing the short channel effect. Ultra-low energy implantation is a crucial process to form shallow junctions. The BED (Boron Enhanced Diffusion) phenomenon, which occurs during high temperature annealing, such as RTA, is a barrier for the shallow junction formation^[1]. Simulating BED as well as TED becomes an urgent task for TCAD. The atomistic model is recognized to be efficient and accurate to include complex mechanism for diffusion simulation. Some good results on atomistic annealing simulation have been published^[2]. And the method has even been applied to the study of CMOS characteristics^[3]. However, study on BED by atomistic simulation has not been presented as we know. In this paper, an atomistic model considering surface emission is proposed to characterize both BED and TED. The RTA annealing at 1000 °C and 1050 °C after boron implantation are simulated. Implantation energy ranges from 0.5keV to 13keV. The simulation results are verified by SIMS data. Agreements between simulation and experiments are achieved. Both BED and TED can be well simulated by the model. The results indicate that the number of boron jumps can be related to the enhancement of diffusion.

II. ATOMISTIC MODEL

A simulator named AMAS (Atomistic Model

Annealing Simulator) is developed based on kinetic Monte Carlo model^[4].

In order to simulate annealing process for ion implantation, a box is defined, which contains all necessary ions and damages. For implantation, the concentration profile is even in lateral direction, i.e. direction perpendicular to that of implantation, except at the edge of implanted field. We just simulate field in the center of implantation window. The width of simulation box is much smaller than that of implantation window. Thus the periodical boundary is applied to the box in lateral direction. And the reduction of box size can save much computing time. However the length of box should be set carefully so that not only the box is long enough for diffusion simulation but also the time cost by computation can be abided. At the same time, an orthogonal mesh is constructed in the box to divide the box into many small cells. Every side of the cell is 2.34 Å long so that the cell take up the average volume occupied by an atom in crystal silicon. The mesh is introduced mainly to simplify the calculations of searching neighbor particles. All particles in box can be mapped on the mesh. So that neighbor particles can be found by checking contents of neighbor cells instead of calculating distance between all particles.

Particles defined in the model are single particles and clusters. Single particles are dopants and point defects. While lattice silicon atoms are excluded. In this paper, boron (B) implantation is studied. Only boron is included as dopant. Point defects include silicon interstitial (I) and lattice vacancy (V). Clusters, including silicon interstitial clusters (I_n), vacancy cluster (V_n) and boron silicon complex (B_nI_m), are defined as the compound of single particles. Possible events of particles are migration, annihilation, combination and cluster evaporation. Migration is the movement of mobile particles, such as I, V and interstitial boron pair (B_i). Annihilation happens between V and I. By combination clusters come into being and grow up. At the same time, clusters evaporate by emitting single particles. All the combination actions of clusters are as follows:

$$I_n + I \rightleftharpoons I_{n+1} \quad (1)$$

$$V_n + V \rightleftharpoons V_{n+1} \quad (2)$$

$$B_n I_m + B_i \rightleftharpoons B_{n+1} I_{m+1} \quad (3)$$

$$B_n I_m + I \rightleftharpoons B_n I_{m+1} \quad (4)$$

Where, for I_n and V_n , $n < 100$ and for $B_n I_m$, $n < 5$ and $m < 5$. The annihilation and combination are assumed to occur whenever two concerned particles are close enough to each other. However, the migration and evaporation happen at a rate determined by energy barrier E_b :

$$\nu = \nu_0 \exp\left(\frac{-E_b}{KT}\right) \quad (5)$$

where E_b is migration energy barrier for migration event or binding energy for clusters evaporation. ν_0 is the attempt frequency and it is generally set as about $10^{13}/s$ which is determined by the thermal oscillation frequency of atoms. The basic parameters used for simulation are shown in table 1.

Table 1. Main parameters for simulation

Events	$\nu_0 (10^{15}/s)$	$E_b (ev)$
V migration	0.0025	0.45
I migration	0.01	0.9
B_i migration	0.01	0.3
$B_i = B + I$	0.01	0.6

The binding energy of In is $2.0 - 1.95(n^{1/2} - (n-1)^{1/2})$ and that of Vn is $2.5 - 2.8(n^{2/3} - (n-1)^{2/3})$ in the unit of ev , n is the size of the cluster. The expression is the fitting to theoretical data^[4] and experimental results. The binding energy of $BnIm$ can be calculated from the total energy scheme presented by Pelaz^[2]. Clusters model is important in explaining TED phenomenon^[2].

The BED is thought to be caused by the emission of Si interstitials from surface^[5]. However what is the source of emission is still under controversy. On the other hand, it is indicated that surface emission should also be considered for TED^[5]. To well simulate both BED and TED, surface emission model is implemented in the simulator. Although boride is indicated to be the possible source of Si interstitial, no special model for boride is considered. In our model, surface is treated as a source and sink for point defects. Defects are trapped at surface and surface emission occurs at the same time. Point defects that are emitted from surface are those that were trapped by surface previously. Thus only defects generated in implantation are included. The rate of surface emission equals to that of annihilation as a simple approximation.

III. RESULTS AND DISCUSSION

The simulation of RTA annealing following boron

implantation is performed. The implantation energy varies from 13keV to 0.5keV. The implantation simulation is carried out by our MD simulator LEACS^[6]. Coordinates of all point defects and dopants are imported into AMAS.

1. Simulation of TED

RTA annealing for 13keV and 5keV boron implantation causes TED. It is simulated to verify the model. The results for 13keV are shown in figure 1. Good agreement between simulation and SIMS data is achieved. TED is obvious in this case.

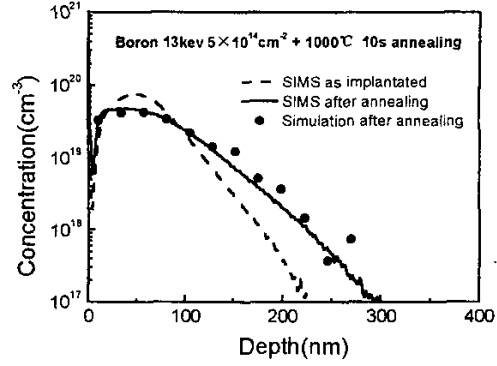


Fig.1. Simulation for 1000 °C 10s annealing after B 13keV implantation.

In order to study the capacity of simulating immobile peak phenomenon in TED, annealing for 5keV implantation with different doses are simulated. The results are shown in fig. 2 and fig.3. It shows that the simulation agree with the SIMS data. There is no obvious immobile peak after annealing for 5keV, $1 \times 10^{15} \text{cm}^{-2}$. While, immobile peak is observed after annealing for $2 \times 10^{15} \text{cm}^{-2}$ as illustrated in fig.3.

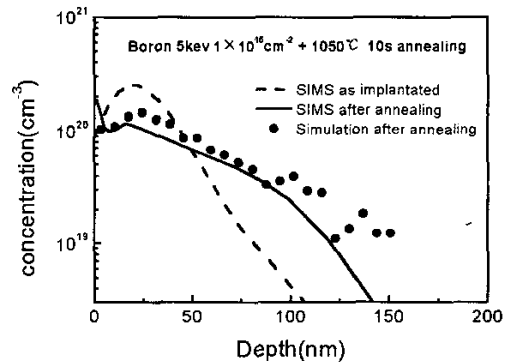


Fig. 2. Simulation for RTA annealing after B implantation with $1 \times 10^{15} \text{cm}^{-2}$ (SIMS data from Ref.[1])

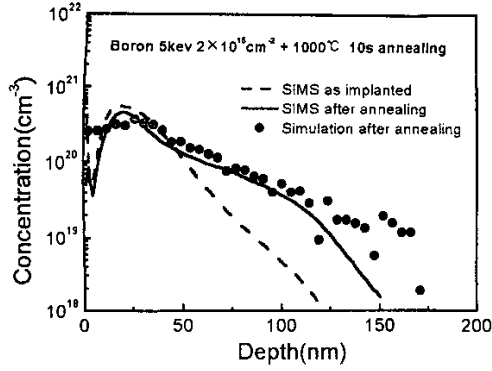


Fig.3. Simulation for RTA annealing after B implantation with $2 \times 10^{15} \text{cm}^{-2}$. Note that immobile peak remains after annealing.

2. Simulation of BED

BED, as reported in Ref.[1], occurs for boron implantation at very low energy. Thus the reported experimental results are simulated by AMAS to verify if the model is valid for BED. The results are shown in Fig. 4. Again, agreements between the simulation and SIMS data are achieved. So the model is capable of simulating BED. It should be pointed out that all the parameters used for here are the same as that for TED simulation presented above. Thus, the model is valid for both TED and BED simulation.

It has been argued that BED is due to surface emission. While it is still not very sure whether surface emission should be included in the explanation of TED. In our model, surface emission is a general model but not a particular model for BED. The simulation presented above indicates that BED and TED can be explained with a uniform model including surface emission.

The BED has been identified for the saturation of diffusivity enhancements at ultra-low energy^[1]. To explain the phenomenon, the total jumps of all boron atoms are extracted from the above simulations. Here, the total jumps are used as the measurement of diffusion. The comparison between the total jumps and diffusivity enhancements is given out in figure 5. It shows that the shape of the two curves agree with each other. Especially that the saturation at energy of 0.5keV and 1keV is represented in simulation results. It indicates that the enhancement of diffusivity can be related to the number of boron jumps. The number of boron jumps can be well traced in the atomistic simulation. In this way, the enhancement of diffusion can be understood better. It indicates that the atomistic model annealing simulation will be more powerful.

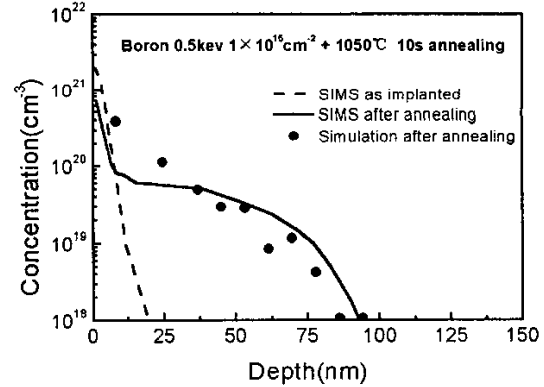
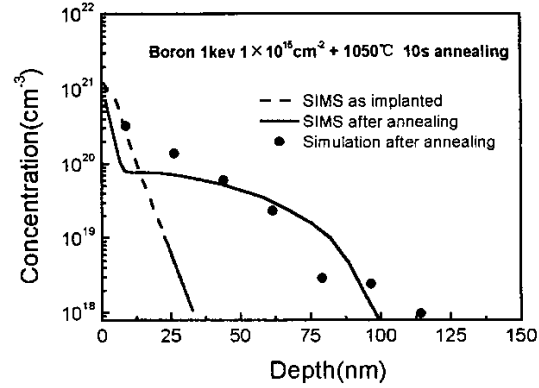
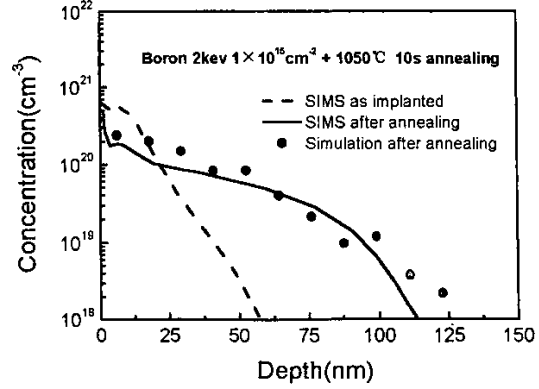


Fig.4. Simulation for the annealing experiments results from Ref. [1] in which the BED phenomenon is identified. Notes that the BED can be characterized by the model.

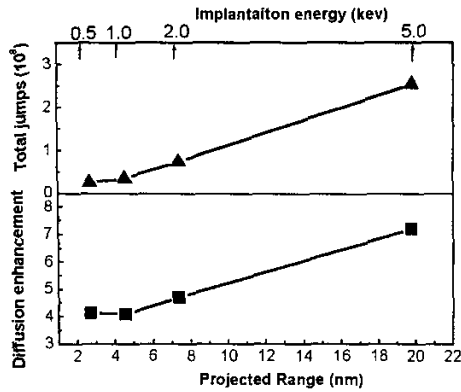


Fig.5. Comparison between diffusivity enhancements and total jumps of boron. The total jumps of all boron atoms in the annealing that symbolized by triangle are extracted from the simulation results presented in fig. 2 and fig. 4. It should be pointed out that the area of implantation window is the same for all simulation examples. The diffusivity enhancements symbolized by square are from Ref.[1], which is extracted from SIMS results. It indicates that the enhancements are related to the number of jumps that borons have performed.

IV. CONCLUSION

An atomistic model considering surface emission to simulate both BED and TED is presented. RTA(1000°C or 1050°C) annealing for B implantation is simulated. The implantation energy covers 0.5keV to 13keV. Simulation results agree with SIMS data. Both BED and TED can be well described. It indicates that BED and TED can be explained with a uniform model including surface emission.

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