Quantum Chemical Molecular Dynamics Simulation of Boron Diffusion and Si Implantation into Silicon Surface

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1. Introduction
Fabrication of forthcoming nanometer scale (<10nm) electronic devices faces many difficulties including formation of extremely shallow and highly doped junctions. At present, ultra-low-energy ion implantation followed by high-temperature rapid thermal annealing is most widely used to fabricate such ultra-shallow junctions. In such process, a great challenge lies in achieving precise control of redistribution and electrical activation of dopant atoms. In the present study, two processes are investigated. One concerns the investigation of dynamic behavior of boron atom in silicon crystal, and the other deals with the process of making shallow amorphous regions near the silicon surface using Si implantation into the silicon surface.

2. Method
The quantum chemical molecular dynamics calculations were carried out using “Colors” program[1,2], which is based on our original tight-binding approximations. This program is over 5,000 times faster than the conventional first-principles molecular dynamics approach.

3. Results and Discussion
3.1 Boron Diffusion in Silicon Crystals
Two models were used for investigating of the boron atom diffusion in silicon crystal (64 atoms). In the first model, one boron atom was put into interstitial site of silicon crystal. In the second model, one silicon atom was removed from the first model to create one silicon vacancy.

In the simulation for the first model, no diffusion of boron atom was observed at 27°C. On the other hand, at higher temperature of 500°C, boron atom diffused through the interstitial sites as shown in Fig. 1, without replacing silicon atom in the lattice site.

In the simulation for the second model, boron atom replaced silicon atom in the lattice, and subsequently, this silicon diffused away to occupy vacancy site as shown in Fig. 2. This behavior was observed at both 27 and 500°C. In order to investigate bonding between silicon and boron, Si-B bond population was analyzed. Fig. 3 shows the time profile of bond population of Si-B. Obviously, one can see that boron forms bond with Si(d) atom at 250 fs and with Si(a) atom at 1100 fs and finally with four different silicon atoms.

Our results indicate that at 500°C boron atom diffuses through interstitial sites in silicon crystal, and boron does not replace silicon atom in the lattice point. When there is a vacancy near the boron atom, which is in an interstitial site of silicon crystal, boron atom first pushes out silicon atom, which is in between boron atom and vacancy to occupy the silicon lattice site. Subsequently, replaced silicon atom at interstitial site diffuses to occupy the vacancy site. This behavior was observed even at low temperature of 27°C.
3.2 **Si Implantation Dynamics into Silicon Surface**

From the quantum chemical molecular dynamics simulation of Boron diffusion (3.1), we found electrical activation of dopants is difficult for low temperature thermal annealing (500 °C) under the condition that boron atom is into interstitial site of silicon crystal. Therefore, one potential measure is to form shallow amorphous region near the silicon surface by implanting Si atom into silicon surface before implantation of boron atoms. The simulation of Si implantation was carried out by using colors program. Fig. 4 shows the snapshots of the molecular dynamics simulation on the Si implantation processes. The initial kinetic energy of Si atom is 1,500 eV and one Si atom was implanted into silicon surface whose area is 1.18 x 10^{13} cm^2, and its impact angle is 90° against silicon surface. This amount of dose corresponds to 8.47 x 10^{13} ions/cm^2. The Si (001) surface was used as a substrate and the dangling bonds were terminated with hydrogen. Furthermore, the substrate consisting of 120 Si atoms and 16 H atoms was used for the simulation, and bottom atoms of the substrate were fixed. Furthermore, the temperature was controlled at 300K by scaling the average velocities of all atoms.

In this simulation, Si atom implanted into silicon surface about 10 fs later and immediately reflected to the atmosphere. The silicon atom that received the direct impact of Si atom moved to the lower direction to occupy the interstitial site of the silicon crystal. The silicon lattice site, which placed impacted silicon atom, remains as a vacancy after Si impact and we can conclude that the so-called partial amorphous region was formed as a result of Si impact. Moreover, simulation of dopant implantation process after making shallow amorphous near silicon surface region are carried out.

In addition to these studies, further different investigations such as impacting angle and kinetic energy of impacting Si atom must be under consideration.

4. **Conclusions**

In the present study, boron atom diffusion in silicon crystal for low-temperature thermal annealing process and simulation of Si implantation into silicon surface to make shallow amorphous regions near the surface was simulated by using “Colors” program. In these simulations, our tight-binding quantum chemical molecular dynamics method was successfully applied to large-scale systems which consider electronic movement. However, future studies to simulate low-energy implantation process using dopant atoms like boron, phosphorus, etc. after making shallow amorphous region near the silicon surface by implanting Si atoms are the matter of interest.

**References**


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**Fig. 4** Dynamic behavior of Si implantation into silicon surface