Extended Abstracts of the 2004 International Conference on Solid State Devices and Materials, Tokyo, 2004, pp. 478-479

**P3-17**

# Depth Profile Prediction on Low Energy Boron Implantation Process by Tight-Binding Quantum Chemical Molecular Dynamics

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## 1. Introduction

In the ultra large-scale integrated circuits, particularly complementary metal-oxide semiconductor (CMOS), the fabrication of ultra-shallow junction is required. In order to realize the boron-doped silicon layers shallower than 50 nm, the ultra low energy implantation technique (less than 1 keV) is regarded as a promising candidate. However, as we suggested in the previous report [1], it seems that the channeling phenomena i.e. diffusion of a doped atom along a [110] direction, become problem when the thickness of the doped layer becomes shallower. Therefore, detailed understanding of the phenomena at the surface during the low energy boron implantation process is important and will promote the practical application of this technique.

In order to analyze the semiconductor processes, computer simulation is an effective and useful method. Among a lot of simulation methods, first-principles static calculation cannot apply to dynamic phenomena at real temperature. On the other hand, first-principles molecular dynamics simulations can simulate dynamic phenomena in principle, but it requires extremely huge computational cost, hence this method cannot be applied to real problems. On the other hand, we have recently succeeded in the development of a tight-binding quantum chemical molecular dynamics program, “Colors”, which is based on our original tight-binding approximations [2-6]. This program is over 5000 times faster than the conventional first-principles molecular dynamics approach. Then, this program enables us to simulate the chemical reaction dynamics at a finite temperature with the consideration of the chemical reaction dynamics using large-scale models that cannot be simulated by the conventional first-principles molecular dynamics approach.

In the previous report [10], we studied the low energy boron implantation process with the boron atom incident along [001] and [110] directions by using the above tight-binding quantum chemical molecular dynamics method, and we have clarified that boron atom tends to diffuse along [110] direction. On the other hand in order to overcome the difficulty of controlling the depth profile of boron concentration for the fabrication of shallow dope layer, inclined incidence of boron atoms is considered to be an effective approach.

In this work, we have succeeded to optimize of the incidence angle of low energy boron implantation processes into silicon surface using our original tight-binding quantum chemical molecular dynamics method.

## 2. Computational Details

A tight-binding quantum chemical molecular dynamics program, “Colors”, which is based on our original tight-binding approximations, is employed to simulate the boron implantation into inclined silicon surface. This pro-

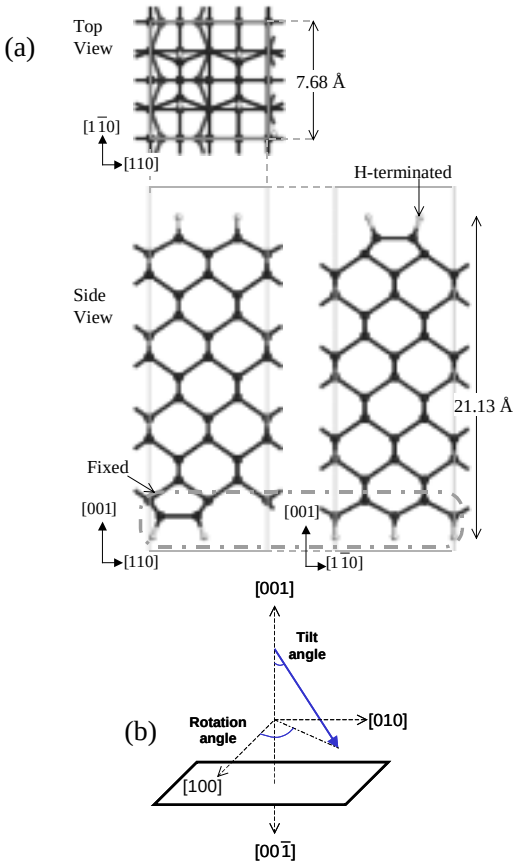


Fig. 1 H-terminated Si(001) 2×1 surface model (a), definition of tilt angle and rotation angle (b)

gram is over 5000 times faster than the conventional first-principles molecular dynamics approach. This program employs various parameters in order to accelerate the calculations, and all the parameters were determined to fit the first-principles calculation results. Hence, this methodology enables us to realize fast and accurate quantum chemical molecular dynamics simulations. The detailed descriptions are reported elsewhere [5-9].

A dimer reconstructed Si(001) 2×1 surface was used as a substrate model (Fig. 1(a)). The surface is terminated by hydrogen atom. The tilt angle and rotation angle used in the present investigations were defined as shown in Fig. 1(b).

In the present study, incident boron atoms with initial kinetic energies of 100 eV were employed. The initial position of boron atom was placed at 7.9 Å above the surface. In addition 98 different (x, y) initial positions of boron atom were chosen for the statistical analysis. All the simulations were performed at 300 K with a time step of $0.1\times10^{-15}$ s.

## 3. Results and Discussion

The boron implantation simulations with tilt and rotation angles were carried out. Fig. 2 shows the typical example of trajectory of the incident boron atom. The results of 98 times simulations are statistically analyzed and are summarized in Table 1. Among the investigated tilt angles shown in Table 1, the average depth increases in the order of 7º < 0º < 22.5º <45º, when the rotation angle is fixed. This result is in good agreement with the experimentally observed phenomena. In order to investigate the influence of rotation angle on the average depth, we have carried out simulations with rotation angle of 45º for tilt angles of 7º, 22.5º, and 45º. The average depths for 45º rotation angle are shallower than those for 0º rotation angle for all the investigated tilt angles. This would be explained by the simulation results that the channeling in [110] direction was suppressed compared to the implantation simulation with rotation angle of 0º. For tilt angles of 7º, 22.5º, and 45º, the ratio of diffusion in [110] direction decreases from 51.3% to 48.4%, from 55.5% to 48.0%, and from 62.5% to 55.3%, respectively. We have theoretically proved the importance of the tilt and particularly the rotation angles in the ultra low energy implantation process.

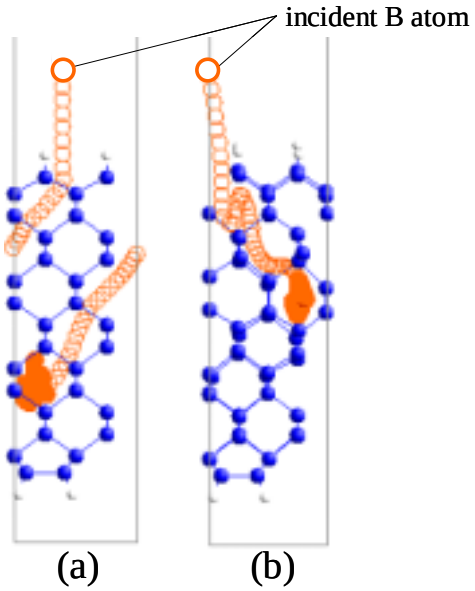


Fig. 2 Typical examples of the incident boron atom trajectory for (a) 0º tilt and 0º rotation angles, (b) 7º tilt and 0º rotation angles.

Table 1, Average depth and diffusion direction of boron atom depending on the incident tilt and rotation angle.

| Tilt angle | Rotation angle | Average depth(Å) | Direction(%) [100] | [110] | [111] |
|---|---|---|---|---|---|
| 0º | 0º | 9.34 | 40.6 | 48.9 | 10.5 |
| 7º | 0º | 8.72 | 41.0 | 51.3 | 7.7 |
| 7º | 45º | 8.66 | 42.8 | 48.4 | 8.9 |
| 22.5º | 0º | 10.84 | 35.7 | 55.5 | 8.8 |
| 22.5º | 45º | 9.91 | 41.6 | 48.0 | 10.4 |
| 45º | 0º | 12.61 | 28.4 | 62.5 | 9.0 |
| 45º | 45º | 10.11 | 32.0 | 55.3 | 12.7 |

## 4. Conclusions

In this study, the inclined implantation of low energy boron into silicon surface was successfully simulated using our original tight-binding quantum chemical molecular dynamics program, “Colors”. We have investigated the influence of tilt and rotation angles on the average depth of dopant. The simulated results well reproduced the experimentally well-known phenomena that the implantation with 7º tilt angle is effective to fabricate the ultra-shallow junction. Furthermore, from the theoretical investigation on the influence of rotation angle, we can predict that the implantation with the rotation angle of 45º will be effective for the fabrication of the ultra-shallow junction.

It was also proved that our “Colors” program is an effective tool to optimize the fabrication processes of ultra-shallow junction or other semiconductor processes that contain chemical reactions.

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