# Molecular Dynamics (MD) Simulation of Ultra-shallow Ion Implantation with a Modified Recoil Ion Approximation

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**Abstract**

In this paper, we report a molecular dynamics (MD) simulation of the ion implantation for nano-scale devices with ultra-shallow junctions. In order to model the profile of ion distribution in nanometer scale, the molecular dynamics with a damage model has been employed. As an exemplary case, we calculate the dopant profile during the ion implantation of B, As, and Ge.

## 1. Introduction

The concentration distribution of dopants during the ion implantation was calculated from the MD approach [1,2]. The MD could accurately calculate the concentration distribution of dopants in the ion implantation using the interaction potentials between atoms.

In this work, in order to model the ultra shallow junction, we used a modified recoil ion approximation for a damage with dose taken into account. The Ziegler-Biersack-Littmark (ZBL) potential model has been used for the interaction among atoms and the distribution of the concentration of dopants were calculated using the potential model - environment-dependent interatomic potential (EDIP) which has been derived from an ab initio database of the cohesive properties of Si in both the diamond and graphite phases.

## 2. Simulation Model

Electronic stopping power is more dominant than nuclear stopping power for low energy ion implantations. In order to model the electronic stopping power, the density functional theory by Echenique *et al* [3] was implemented in this work. Furthermore, the Firsov model was employed in order to model the energy loss during the inelastic collisions [4]. The channeling effect is taken into account during ion implantation even at low energy. Although ions are implanted in target atoms with low energy, the shallow junction depth cannot be obtained because energetic ions diffuse freely through the channels, if channels are made in the target atoms. In order to restrain the channeling effect, we should increase the ion dose and control the tilt angle into the target atoms. So a good result could be obtained.

## 3. Results and Discussion

In the simulations, the crystalline silicon was used as a target material. The simulation was performed at 300 K. A beam divergence of 1° was used in all simulations. The number of simulated ions was 10000, which is enough to obtain good statistics in the profile. Implantations in a random direction were done in simulations by tilting the azimuthal angle of the implantation with 6~7 degrees off the <110> surface normal. In the simulations, the dopants were B, As and Ge ions. Overall good agreements with experimental data were obtained in the simulations. The range distribution agrees with the SIMS data.

As the implantation energy increases, the electric characteristics of semiconductor devices are improved in the wide distribution of dopants. However, we had difficulty in obtaining the shallow junction depth. Small and light ions like B caused less lattice damage near the surface at high implantation energy. But at the depth of the target material when ion energy is gradually decreased, nuclear stopping power is more dominant than electronic stopping power and a lot of lattice damage occurred. The concentration distribution difference in the deeper region increases because ions were scattered to sides due to the collisions with lattice damages. On the other hand, heavy

ions like As and P cause much lattice damage near the surface.

All simulations were performed on a Si {100} target at a temperature of 300K. Dopants and damage profiles were simulated for B, As, and Ge ions with the dose $1\times10^{14}$ ions/cm$^2$. Fig.1 shows the simulation results with the energy of 0.5, 1, 2, 4, 8, 16 keV B implant into Si. In case of Fig. 2 and Fig. 3, the implant ion is As and Ge, respectively. Table 1 shows the parameters of EDIP for silicon.

As boron ion dose increase, local damage accumulation much affects dopant distribution in the cases of ultra-low energy ion implantation, i.e. the channeling tail drop very steeply with dose increase. In case of As ion, the channeling tail drops very steeply with depth. This phenomenon is due to the large atomic mass of arsenic ion.

## 4. Conclusions

In conclusion, the EDIP model was employed for the MD simulations, which exhibited a good agreement with the ones with empirical potential models. In order to model the shallow junction depth, we prove the accuracy of dopant concentration distributions including B, As and Ge at low energy for nano-scale device fabrication.

## References

[1] J.Nord, *et al,* Phys. Rev. B (2002).

[2] J. Peltola *et al.*, Nucl. Instr. Meth. Phys. Res. B, (2002).

[3] P. M. Echenique et al., Appl. Phys. A 71, 503 (2000).

[4] P. Keblinski *et al,* Phys. Rev. B 66, 4104 (2002).

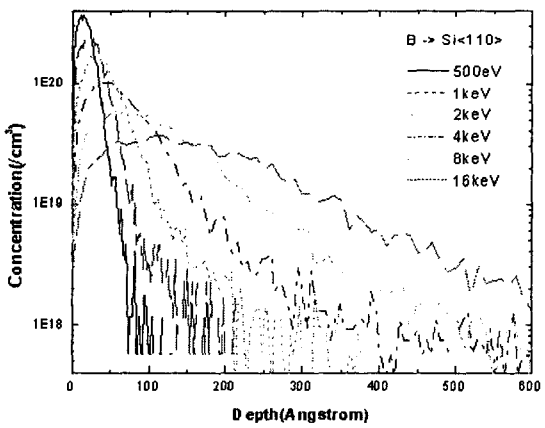


Fig. 1 A plot showing the simulation results with the energy of 0.5, 1, 2, 4, 8, 16 keV and the dose $1\times10^{14}$ions/cm$^2$ B implant into Si<110>.

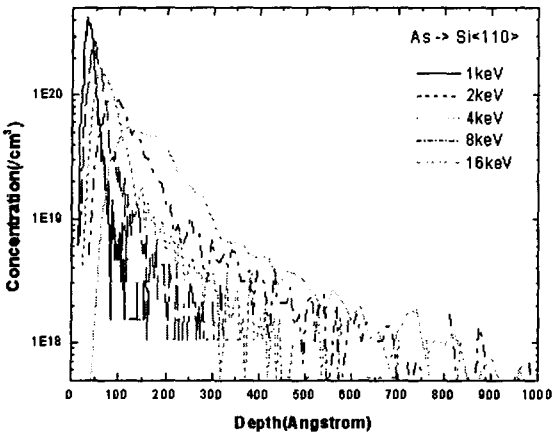


Fig. 2 A plot showing the simulation results with the energy of 1, 2, 4, 8, 16 keV and the dose $1\times10^{14}$ions/cm$^2$ As implant into Si.

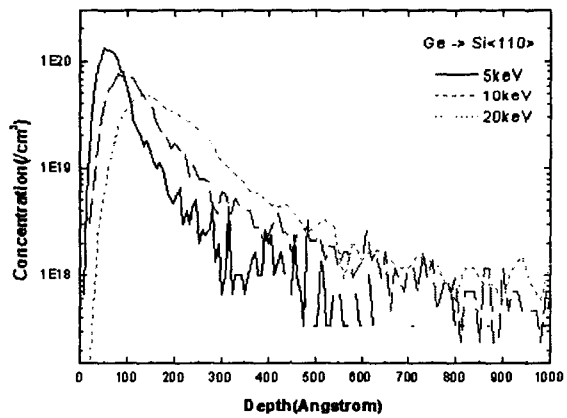


Fig. 3 A plot showing the simulation results with the energy of 5, 10, 20keV and the dose $1\times10^{14}$ions/cm$^2$ Ge implant into Si.

Table 1. Parameters of EDIP for silicon

| Parameter | Value | parameter | value |
|---|---|---|---|
| A | 7.9821730 eV | $\gamma$ | 1.1247945 Å |
| a | 3.1213820 Å | $\mu$ | 0.6966326 |
| $\lambda$ | 1.4533108 eV | $\rho$ | 1.2085196 |
| $Q_0$ | 312.1341346 | $\sigma$ | 0.5774108 Å |
| $\alpha$ | 3.1083847 | $\eta$ | 0.2523244 |
| B | 1.5075463 Å | $\beta$ | 0.0070975 |
| c | 2.5609104 Å | | |