Extended Abstracts of the 2004 International Conference on Solid State Devices and Materials, Tokyo, 2004, pp. 482-483

P3-19

Molecular Dynamics (MD) Calculation for Low-energy Ion Implantation Process with Dynamic Annealing Effect

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1. Introduction

In this paper, we report a molecular dynamics (MD) simulation on the ion implantation for nano-scale CMOS 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 with the Kinetic Monte Carlo (KMC) diffusion model used for the dynamic annealing between cascades. The concentration distribution of dopants during the ion implantation was calculated using the interaction potentials between atoms [1,2] from MD calculation.

2. Numerical Models

In this work, the concentration distribution of dopants during the ion implantation is calculated with MD approach. The MD approach accurately calculates the concentration distribution of dopants in the ion implantation using the recoil interaction approximation (RIA). MD simulations can predict range profiles of different ion species implanted into crystalline Si for nano-scale CMOS devices in ultra low energy regime. In our work, MD with a damage model has been employed. In order to model the ultra shallow junction, a modified RIA is used for dose-dependent damage. The Ziegler-Biersack-Littmark (ZBL) potential model was used for the interaction between atoms. In order to model the electronic stopping power, the density functional theory by P. M. Echenique [3] was implemented in this work. Furthermore, the Firsov model was employed in order to take the energy loss during the inelastic collisions into account [4]. For the consideration of dynamic annealing during ion implantation between cascades, KMC diffusion is performed with MD calculation. From the atomic distribution during the ion implantation from MD simulation, the dynamic development (hopping) of impurities and defects are calculated through KMC calculation. The KMC simulation is interactively performed with the results of the MD simulation.

3. Simulations

All simulations were performed on a Si {100} target at 300K. Fig. 1 shows the calculation results for B implant with the energies of 1, 3, and 5keV, respectively, with dose of 1×10^{14}ions/cm^2 into Si. The tilt and rotation angle is '0'. In case of 1keV ion implantation, the peak is observed near at the surface when compared with the case of the energy of 5keV, while the end of range is deeper than that of the energy of 1keV. The mean range of the ion implantation with the energy of 1keV is 2.7nm. This seems to be due to the fact most of the implantation energy is lost during the bombardment with surface atoms. The maximum range of ion implantation with the energy of 5keV is 87nm, which is about 4.3 times deeper than the case with the energy of 5keV. It looks like that the difference is due to the degree of amorphization of the surface and the more significant energy loss of 5keV when compared with the energy of 1keV. Fig. 2 illustrates boron implant with energy of 5keV with the dose of 1×10^{14}ions/cm^2 and 1×10^{15}ions/cm^2 into Si, small dose dependence. However, if there is more dose difference, the results similar to the one shown in Fig.1 may be obtained.

Fig. 3 shows the simulation results for B, for energies down to 100eV below 10keV, and Fig. 4 shows the mean range and the sputter energy per ion. In the range below 1keV, the peak is located near the surface down below 2.5nm, and the most atoms are within the range of 10nm. Fig. 5 and Fig. 6 demonstrate the simulation results for B implant with energy of 15keV, the dose of 1×10^{15}ions/cm^2, and the dose rate of 1×10^{12}ions/cm$^2\cdot$sec with taking dynamic annealing into account. The Si target experiences the amorphization after 384 sec. The thickness of amorphous layer is about 90 nm after 1000 sec. Fig. 7 illustrates B and interstitial profiles with energy of 3keV, the dose of 1×10^{14}ions/cm^2, and the dose rate of 1×10^{12}ions/cm$^2\cdot$sec both with and without dynamic annealing into account, respectively. Boron migrates to the target surface due to the dynamic annealing, while the peak value of interstitial with the dynamic annealing is lower than that without the dynamic annealing due to recombination with vacancy. Fig. 8 and Fig. 9 illustrate comparison of our simulated B profiles with UT-MARLOWE and SIMS profiles. The B profiles with the dynamic annealing give quite good agreement with SIMS profiles.

4. Conclusions

The dopants, interstitials, and vacancies distributions have modeled and calculated by using molecular dynamics with the dynamic annealing. The dopant profiles have been changed due to the diffusion with interstitials and vacancies between cascades of ion. For the energy of 2keV and the dose of 1×10^{14}ions/cm^2, the implanted B profiles with the dynamic annealing give quite good agreement with UT-MARLOWE and SIMS profiles.

References

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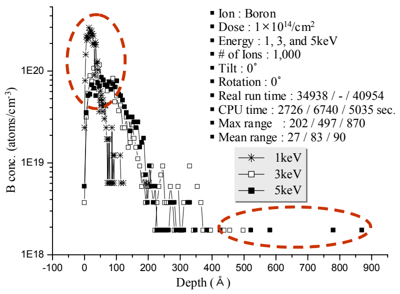


Fig. 1 A plot showing the simulation results for B implant with the energies of 1, 3, and 5keV and the dose of 1×10^{14} ions/cm^2 into Si.

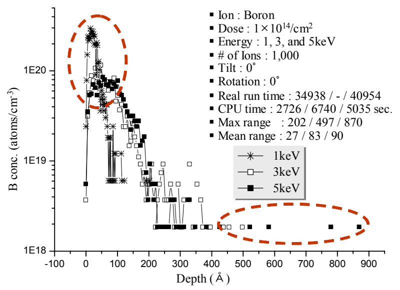
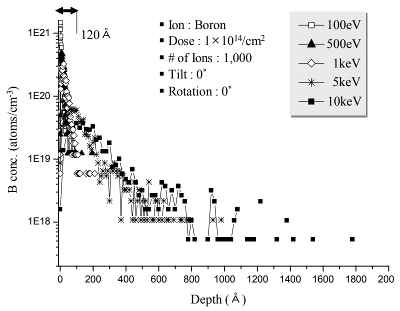
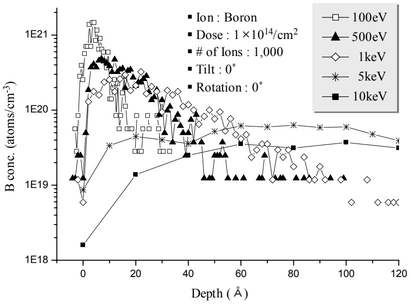


Fig. 2 A plot showing the simulation results for B implant with the dose of 1×10^{14}ions/cm^2 and 1×10^{15}ions/cm^2 and the energy of 5keV into Si.



(a)



(b)

Fig. 3 Plots showing (a) the profile and (b) the profile in the range of 12nm of B implant with the energy of 100eV, 500eV, 1keV, 5keV, and 10keV into Si.

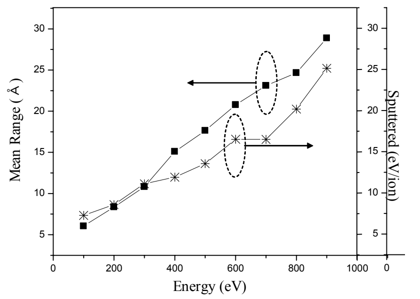


Fig. 4 A plot showing the mean range and the sputtered atoms for B implant with the energies down to 100eV below 1keV and the dose of 1×10^{14}ions/cm^2 into Si.

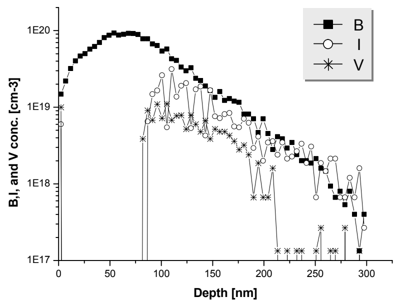


Fig. 5 A plot showing the simulation results for B implant with the energies of 15keV, the dose of 1×10^{15}ions/cm^2, and the dose rate of 1×10^{12}ions/cm^2·sec with dynamic annealing.

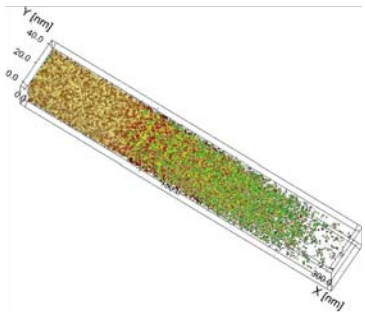
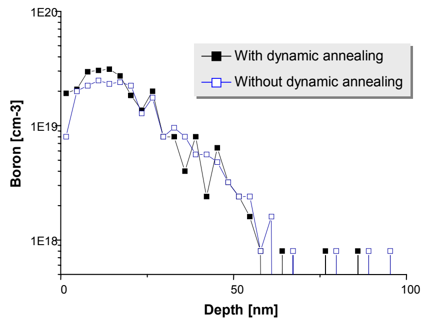
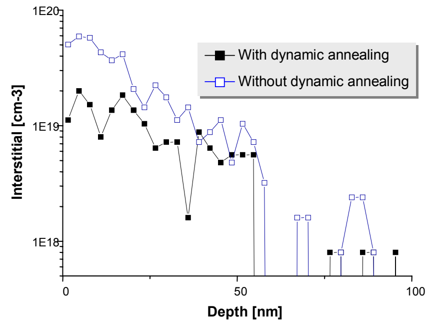


Fig. 6 A plot showing (a) the particle distribution after 384 sec. and (b) 1000 sec with the condition of Fig. 5.



(a)



(b)

Fig. 7 Plots showing (a) B profile and (b) interstitial profile with the energies of 3keV, the dose of 1×10^{14}ions/cm^2, and the dose rate of 1×10^{12}ions/cm^2·sec with and without dynamic annealing.

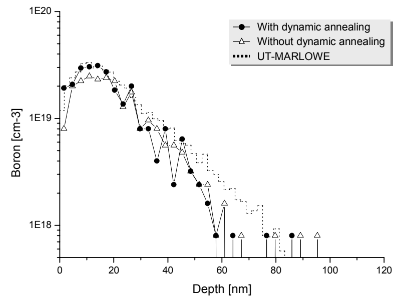


Fig. 8 A plot showing the comparison of B profiles with the condition of Fig. 7.

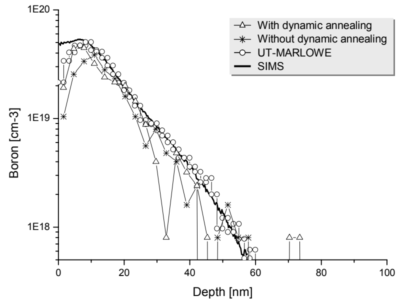


Fig. 9 A plot showing the comparison of B profile with the energies of 2keV, the dose of 1×10^{14}ions/cm^2, and the dose rate of 1×10^{12}ions/cm^2·sec with dynamic annealing.