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Atomistic Modeling for Boron Up-Hill Diffusion After Ge Pre-Amorphization

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INTRODUCTION

Pre-amorphizaing implants (PAI) are a promising option for forming highly doped B ultra shallow junctions [1]. With increasingly stringent requirement on source/drain extension junction depth scaling in CMOS devices, pre-amorphization has also been used prior to low energy implant to generate shallower junction depth [2].

In this work, we investigated the effect of Ge pre-amorphization on low energy B implant and up-hill diffusion mechanism due to excess interstitials at EOR using Kinetic Monte Carlo (KMC) for the first time

RESULTS and DISCUSSTION

For investigating Ge PAI effect, Ge implantation is performed with dosage varying from 5 x 10^{12} to 5 x 10^{15}/cm^2 and with an implantation energy varying from 10 to 50 keV. Further, B implantation is performed with dosage of 1 x 10^{15}/cm^2 and implantation energy 0.5 and 1.5 keV.

Figure 1 shows the comparison KMC data with SIMS data for accounting the Ge PAI effect. In this figure, diffusion profiles are in good agreement with experimental data. Figure 2 shows the diffusion profile with varying Ge implantation energy. We can see that implantation energy of Ge does negligible influence on the uphill-diffusion of boron. In addition, figure 3 shows the diffusion profile with varying dose of Ge. With increasing the dose of Ge 5 x 10^{12} to 5 x 10^{15}/cm^2, uphill-diffusion effect also increases.

One of the up-hill diffusion mechanisms in PAI silicon is the flux of self-interstitials from the EOR defect band. During thermal annealing, point defects vanish from amorphous region by I-V recombination. As a consequence, interstitial flux to the surface occurs and this phenomenon is an important effect of "up-hill" diffusion which reduces boron TED and minimizes the junction depth [1]. Figure 4 explains this mechanism. In order to confirm this mechanism, we simulate self-interstitials in terms of very low time scale. Figure 5 shows the interstitial profile without Ge PAI and figure 6 shows the interstitial profile with Ge PAI. In figure 6, we can see the difference of surface density of interstitials with bulk density of interstitials, but not in figure 5. Therefore, the flux of interstitials towards surface is observed in the Ge PAI.

In our KMC simulations, the parameters were obtained either from ***ab-initio calculation*** or from experimental data. Figure 7 shows the migration and binding energies employed in this study. [3, 4].

CONCLUSION

In this work, the boron diffusion in the Ge pre-amorphized silicon was simulated in the atomistic scale. Our KMC simulation profiles of boron in PAI silicon were compared with experimental data and excellent agreement was confirmed. Also we can see the key mechanism of uphill diffusion through simulating interstitials using KMC method. Furthermore, we also confirmed that boron TED could be reduced from using the Ge PAI. These techniques are useful for reducing boron TED and thus seem to be very effective for obtaining the ultra shallow junction for PMOS devices.

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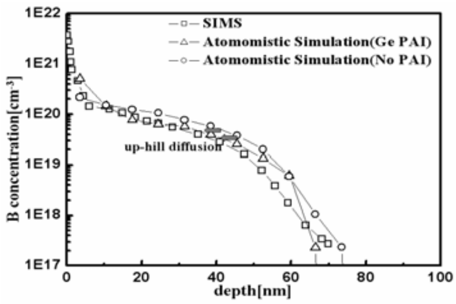

Fig. 1. Comparison with SIMS data and up-hill diffusion effect; boron 0.5 keV, 1 x $10^{15}/cm^2$, germanium 10 keV, 1 x $10^{15}/cm^2$ and 1000 ℃ 10s (RTA).

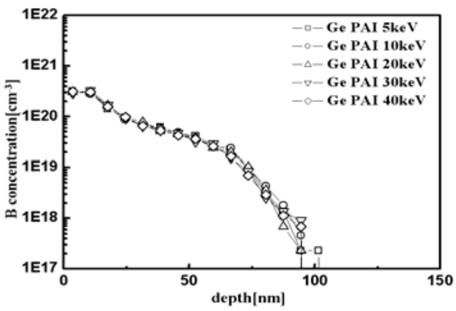

Fig. 2. Boron profiles are compared with Ge PAI wherein energy varies from 5 keV ~ 40 keV ; boron 1.5 keV, 1 x $10^{15}/cm^2$ and 1000 ℃ 10s (RTA).

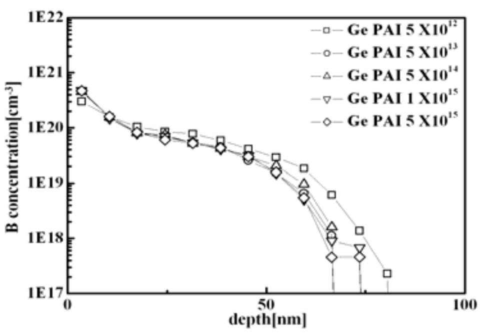

Fig. 3. Boron profiles are compared with Ge PAI wherein dosage of Ge varies from 5 x $10^{12}/cm^2$ ~ 5 x $10^{15}/cm^2$; boron 0.5 keV, 1 x $10^{15}/cm^2$ and 1000 ℃ 10s (RTA).

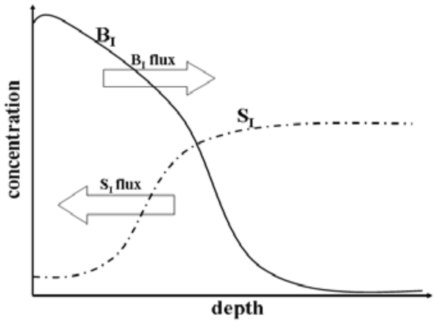

Fig. 4. This figure shows "up-hill" diffusion mechanism

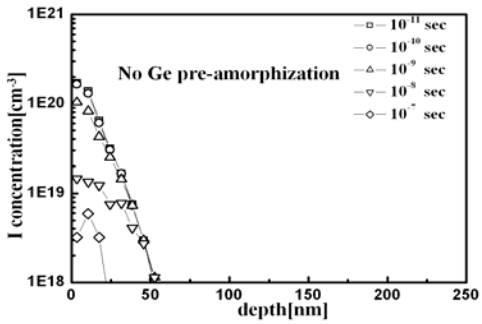

Fig. 5. Interstitial profiles in terms of very low time scale with no Ge PAI

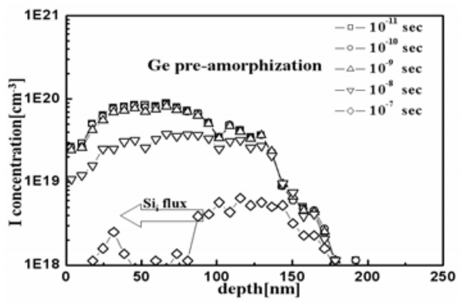

Fig. 6. Interstitial profiles in terms of very low time scale with Ge PAI

	B_2I_3 =-6.0	B_3I_3 =-8.0	B_4I_3 =-8.5
BI_2 =-3.3	B_2I_2 =-4.6	B_3I_2 =-6.0	B_4I_2 =-6.5
	B_2I =-1.6	B_3I =-3.6	B_4I =-4.0
	B_2 =0.8	B_3 =0.8	B_4 =0.8

Fig. 7. Migration and binding energies of B_mI_n clusters use in this work.