Three-dimensional Modeling of the TED due to Implantation Damage

Jaehee Lee, Sangho Yoon, Yountae Kim, Taeyoung Won, Jongchoul Kim*, and Daehun Lee*

Inha Research Institute of Semiconductor and Thin Film Technology
School of Electrical and Computer Engineering, Inha University
253 Younghyun-Dong, Nam-Ku, Inchon, 402-751, KOREA
E-mail: ljh@hsel.emde.inha.ac.kr FAX: +82.32.862.1350
*Memory R&D Division, Hyundai Electronics Industries, Co., Ltd.

Abstract -- In this paper, we report the three-dimensional simulation result of the transient enhanced diffusion(TED) of dopants in the ion implanted silicon by employing our 3D semiconductor process simulator, *INPROS* system. In order to simulate three-dimensional TED redistribution of dopants in the silicon, the defect distributions after ion implantation was calculated by plus one model, followed by finite element numerical solver for thermal annealing. Our three-dimensional TED simulation could successfully interpret the pile-up phenomena by modifying the diffusion model to the pair-diffusion model. Excellent agreement between the simulated 3D profile and the SIMS data has been obtained.

I. INTRODUCTION

In the recent VLSI technologies, thermal budgets have been greatly reduced in an effort to prevent the dopant redistribution in thermal processes such as gate oxidation, nitridation, and annealing. However, the anomalous diffusion of dopants were observed even at low temperature process followed by the ion implantation[1][2][3]. This phenomenon, which is called implant damage induced transient enhanced diffusion, is due to the enhanced diffusivity of dopants in the vicinity of the ion-implanted region with a large amount of point defects. Since the situation gets worse in the case of the amorphization of the implanted source/drain(S/D) regions, it is invaluable to understand the physical mechanism of TED and develop a numerical simulation tool in order to control the TED effects for the next generation CMOS process[5][6]. In this paper, we report the implementation of a 3D TED process simulation program into the framework of the *INPROS(Inha Process Simulator)* system.

II. SIMULATION MODEL

The 3D INPROS diffusion module includes a diffusion and recombination model of point defects, and a defect-dependent diffusion model of various dopants by solving the 3D coupled diffusion equations in finite element method. To account for the pile-up of dopants at the surface, the dual diffusion model was modified to the pair diffusion model. And for the generation of point defects, the "plus one" model was chosen. The interstitial-vacancy pair dose not seem to affect the diffusion of dopants much because of its rapid recombination after the ion implantation. However, the silicon interstitials generated by the implanted ions enhance the diffusivity of dopants. In the case of high energy implantation, the silicon interstitial does not seem to affect the diffusivity of dopants at the beginning of the annealing due to the formation of the clustering of the interstitials. However, the transient enhanced diffusion can be observed instead as the relaxation continues with time[2][3].

After the three-dimensional distribution of the silicon interstitial was calculated by the Monte Carlo method, the effect of the implant species and dosage of implanted ion on the TED behavior of dopants was investigated by solving the coupled diffusion equations numerically. In order to observe the redistribution of the dopants due to the point defects generated by the ion implantation, the three-dimensional distribution of point defect in an epitaxially grown boron marker layer after the ion implantation was calculated by Monte Carlo method. After the phosphorus/ arsenic implantation, numerical simulation of N_2 annealing @750 °C for 30~120 minutes was performed. To investigate the reversed short channel effect(RSCE) phenomena, the TED model was applied to the 0.35 micron CMOS process.

III. RESULTS

In Figure 1 is shown the distribution of dopants after annealing the boron marker layer implanted with a dose of 1×10^{14} cm^{-2} of phosphorus for 50 keV @750 °C for 2 hours. The simulation results revealed that the redistribution of dopants does not occur at all even for the annealed marker layer if the marker layer did not undergo severe point defect generation. In addition, the calculated diffusion profiles of boron and phosphorus exhibited the strong dependence of their diffusvities on the generated silicon interstitials. In Figure 1, the simulation results of two types of diffusion model, the dual-diffusion model and the pair-diffusion model are compared with the SIMS data. The broadening of the buried channel profile in the vicinity of the ion implanted region can be explained by relying on the dual-diffusion model:

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$$\frac{\partial C}{\partial t} = \nabla (D_I \left(\frac{C_I}{C_I^*}\right) \nabla C) \qquad (1)$$

Since the dual-diffusion model simply calculates the enhancement of diffusivity according to the amount of point defects, the effect of pile-up of dopants due to defect flux from a substrate to the surface is not taken into account in the model. At the gate oxide interface, the damage decreases steeply from a peak to a low value by interstitial recombination. Such a retrograde profile of point defects causes a boron pile-up at the surface. This phenomena can be included to the diffusion model by modifying to the pair-diffusion model:

$$\frac{\partial C}{\partial t} = \nabla (D_I \left(\frac{C_I}{C_I^*}\right) \nabla C + D_I \left(\frac{C}{C_I^*}\right) \nabla C_I) \qquad (2)$$

In Figure 1 is shown the calculated profile of phosphorus exhibiting the pile-up at the surface.

In the meanwhile, as shown in Figure 2, arsenic ions do not seem to redistribute their profile according to the silicon interstitials because their diffusion is more affected by silicon vacancies than silicon interstitials. Figure 1 and 2 show simulated profiles together with the experimental point data of SIMS profiles[2] of boron, phosphorus and arsenic. It can be seen that the agreement is quite good for the above species of dopants. In Figure 3 is shown the profiles of the redistributed dopants for various annealing temperatures. It can be seen that the redistribution of the implanted dopants is more pronounced when the annealing temperature is below 900℃. This seems to be due to the fact that the low equilibrium concentration of defects with reduced annealing temperature decreases the recombination rate of point defects.

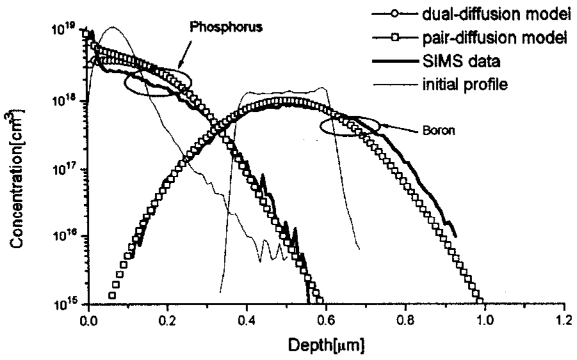

Fig. 1 Boron profiles after implanting phosphorus with a dose of 1×10^{14} cm^{-2} and an energy of 50 keV, followed by annealing at 750 ℃ for 30 minutes.

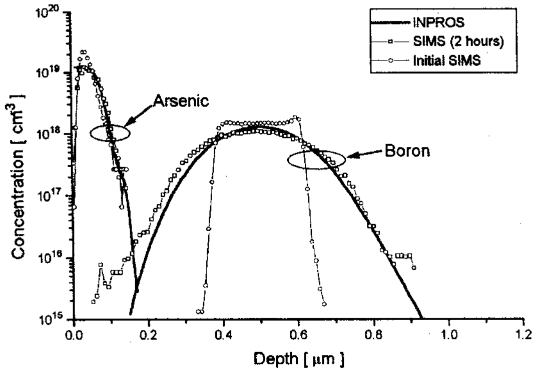

Fig. 2 Boron profiles after implanting arsenic with a dose of 1×10^{14} cm^{-2} and an energy of 50 keV, followed by annealing at 750 ℃ for 2 hours.

It is well known that the reverse short-channel effect (RSCE) is attributed to excess point-defect generation due to source/drain implantation. The RSCE deteriorates the reliability of the scaled devices due to the fluctuation of the threshold voltage. The TED model of dopants was applied to the CMOS process to investigate the RSCE phenomena. An LDD structure was formed by implanting a dose of 1×10^{15} cm^{-2} of arsenic at an energy of 200 keV, and 1×10^{13} cm^{-2} of arsenic at an energy of 50 keV, respectively. A V_T adjustment was conducted by implanting a dose of 1×10^{12} cm^{-2} of boron at 40 keV, followed by annealing at 750℃ for 30 minutes. In Figure 4 is shown the three-dimensional TED redistributed profile of boron. As shown in Figure 4, transient enhanced diffusion due to ion implantation process at the edge of the gate can cause impurity to diffuse out to the surface and broaden the impurity profile. In Figure 4 and 5 are shown the three dimensional distribution of generated interstitials due to ion implantation of arsenic atoms.

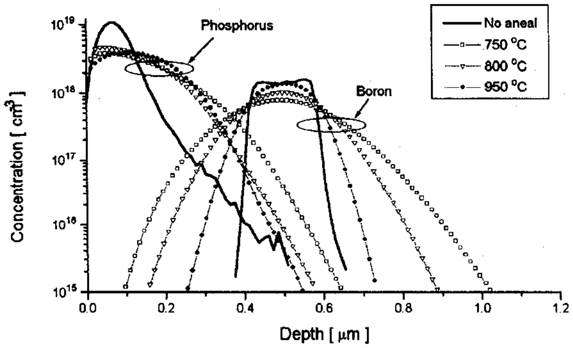

Fig. 3 The redistributed profile of boron and phosphorus when annealing temperature is varied from 750, 800 and 900℃.

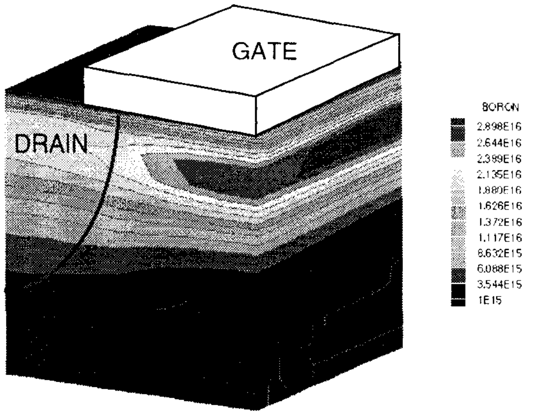

Fig. 4 Three-dimensional contour of boron after the implantation of a dose of 1 × 10^{15} cm^{-2} of arsenic at an energy of 200 keV, and 1 × 10^{13} cm^{-2} of arsenic at an energy of 50 keV, respectively, and followed by annealing at 750℃ for 30 minutes.

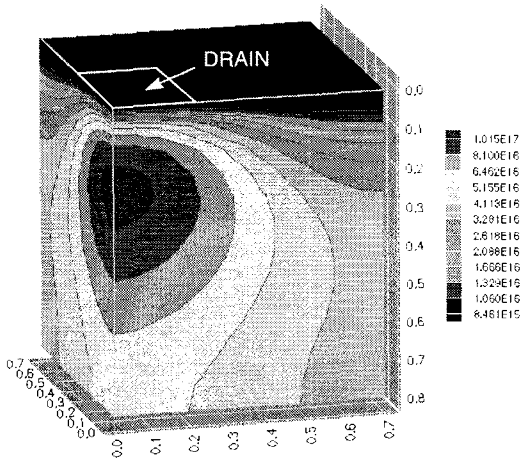

Fig. 5 Three dimensional distribution of interstitials generated due to the ion implantation of arsenic atoms after annealing at 750℃ for one minute.

At the interface of silicon/oxide, the recombination of interstitial is more rapid than at the bulk causing impurity out-flux to the surface. As the amount of generated interstitials near the surface region is reduced, the effect of the transient enhanced diffusion is greatly reduced.

IV. CONCLUSIONS

Our three-dimensional TED simulation shows excellent agreement between the simulated 3D profile and the SIMS data has been obtained. The simulation results revealed that the redistribution of dopants does not occur at all even for the annealed marker layer if the marker layer did not undergo severe point defect generation. In addition, the calculated diffusion profiles of boron and phosphorus exhibited the strong dependence of their diffusvities on the generated silicon interstitials. The effect of pile-up of dopants due to defect flux from a substrate to the surface is taken into account in the pair-diffusion model.

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