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Ion implantation into multi-layer targets is simulated by using the Monte Carlo method, considering recoil process. In this calculation, the target atom that acquired a threshold energy during a collision, is tracked as well as the implanted ion. Characteristic features of oxygen atoms recoiling from the surface oxide layer into silicon are investigated.

Ion implantation is still widely used for introducing dopant into silicon substrate. In practical device fabrication, implantation is frequently carried out on a substrate which is covered with one or more layers such as  $SiO_2$ ,  $Si_2N_4$ , or  $WSi_2$ . In such occasion, for example, the recoiled oxygen becomes an origin of Icakage current, and suppresses the implantation-induced-dopant-enhanced-diffusion[2]. Hence, a model of atom recoiling occupies a significant part in the modern critical process simulation.

The oxygen distribution recoiling from the oxide layer on the silicon surface was simulated by tracking collision cascade based on the Monte Carlo method[3,4]. Although channeling effect in crystal silicon can be simulated by taking into account the crystal structure with the target atom thermal vibrations[5], the following results were obtained by assuming the amorphous target material.

Figure 1 shows the simulation results for arsenic ion implantation into silicon through a  $550\text{\AA}$ -thick SiO<sub>2</sub> layer. Both arsenic and recoiled oxygen concentration agree with the experimental data[1], which were also reproduced by the Boltzmann transport equation method[6]. Figures 2 show the two components of the total recoiled oxygen distribution where the  $300\text{\AA}$ -thick oxide layer was divided into five  $60\text{\AA}$ -thick sub-layers. Figure 2(a) shows the oxygen distribution when recoiling takes place only at the top surface layer (region A), while in Figure 2(b), only at the inside  $60\text{\AA}$ -thick oxide layer (region B). The concentration of oxygen originating from the surface layer is smaller than that from the inside layers. However, since the high energetic collisions are likely to occur relatively near the surface region, the oxygen distribution spreading in Fig.2(a) is larger than that in Fig.2(b). This result indicates that surface contaminants can recoil deep into the substrate during implantation which may result in possible higher leakage current.

In conclusion, the recoil atom distribution in a multi-layered target has been simulated. The useful information could be obtained by using a precise Monte Carlo method, for the ion implantation process.

References

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Figure 1. Simulation results for the implantation of 180 keV As into silicon through a 550Å-thick SiO<sub>2</sub> layer, compared with the experimental results by llirao[1].



Figure 2. Simulation results for 100keV As implantation into silicon through a 300Å-thick SiO<sub>2</sub> layer. The oxide layer was divided into five 60Å-thick sublayers. (a) Oxygen distribution (broken line), recoiling from top 60Å surface sub-layer (region A). (b) Oxygen distribution(broken line), recoiling from the inside 60Å-thick sub-layer(region B).