Extended Abstracts of the 19th Conference on Solid State Devices and Materials, Tokyo, 1987, pp. 295-298

Two-Dimensional Monte Carlo Simulation of Damage Distribution Induced by Ion Implantation into Submicron Silicon Areas

Shoji Shukuri, Tohru Ishitani, Masao Tamura and Yasuo Wada
Central Research Laboratory, Hitachi, Ltd.
Kokubunji, Tokyo 185, Japan

A two-dimensional distribution of damage was calculated by using a Monte Carlo program with the Kinchin-Pease equation for ion implantation into submicron areas of Si. Simulated results predict that damage profiles have strong mask size dependences. This is considered to play an important rule in secondary defect growth during thermal processes after implantation. The two-dimensional distribution of the damage and secondary defects in focused boron ion beam implanted Si layers was evaluated using a cross sectional SEM and TEM observation. The experimental results of the damage profiles provided qualitative agreement with those of the simulations.

1. Introduction

Continuous demands for the miniaturization of the element devices in Si LSI have led to the development of finer and shallower junction formation techniques. With the reduction in junction size, it has become more important in designing junctions to precisely know the two-dimensional distributions of primary damage and impurities.

In this paper, the two-dimensional distribution of damage in ion implanted submicron Si areas are simulated by a Monte Carlo program. Focused ion beam (FIB) implanted Si layers are evaluated by utilizing cross sectional SEM and TEM observations. Experimental results are discussed in comparison with the simulated ones.

2. Monte Carlo Simulation

A. Simulation program --- The Monte Carlo program developed by Ishitani [1] was used to follow the three-dimensional trajectory of the energetic ions in amorphous Si substrate as well as to calculate the primary displacement energy transferred to the lattice atoms. In this program, the two-body collision model is employed, and the two-body interaction potential is the Moliere type [2]. To simulate the three-dimensional distribution of primary damage due to ion implantation at one below the surface, incident ions of 4×10^{5} were used with fixed incident energy.

B. Primary damage calculation --- The distribution of Frenkel pairs was calculated using the Kinchin-Pease equation [3]. The total number of Frenkel pairs produced by the primary nulear energy transfer was determined from

$$\nu = 1 \quad \text{for } E_d < E_\nu < 2.5E_d,$$
$$\nu = 0.8E_\nu/2E_d \quad \text{for } 2.5E_d < E_\nu \qquad (1),$$

where E_ν and E_d are the transfer energy of the nuclear collision and the displacement energy, which is approximately 25 eV, respectively. The two-dimensional distribution of Frenkel pairs in ion implanted submicron region can be calculated by superposing the three-dimensional distributions of damage to single ion implanted points. A Gaussian profile with a standard deviation of $\Phi/2\sqrt{2}$ was assumed for the FIB, where Φ is the beam diameter.

3. Experimental Procedures

A. Focused boron ion beam implantation --- A 100keV FIB implantation system equipped with a liquid metal ion source and electromagnetic mass separator was utilized in this work. A 70keV B^+ FIB with a diameter of 0.2μm was line-scanned over a Si substrates. The line doses were varied between 2×10^{10} and 2×10^{12} ions/cm.

B. Characterization of primary damage profiles --- The two-dimensional distribution of the damage in Si was evaluated by the chemical etching of a cross section of the FIB-implanted layers. The Wright etchant [4] was employed to etch the damaged region. After the etching, an SEM (Hitachi S-800) was used to observe the etched contours. TEM observation was also employed to evaluate the two-dimensional distribution of the secondary defects that resulted from the thermal annealing after implantation.

4. Results and Discussions

A. Monte Carlo simulation ---The normalized two-dimensional distributions of Frenkel pairs for ion implantation of a point at 70keV are shown in Fig. 1. The maximum Frenkel pair concentration region existed at the Si surface. The average energy transferred to primary displaced atoms by the 70keV boron ion implantation was calculated [5], and its maximum value was 0.5keV. The approximate depth for the Si^+ ion implantation into Si at 0.5keV is about 0.5nm. This fact indicates that the Frenkel pair profiles calculated by the Kinchin-Pease equation are reasonably accurate for B^+ ion implantation.

The normalized two-dimensional Frenkel pair density contours for B^+ ion implantation are compared in Figs 2(a) and (b). Implantation with a 70keV FIB having a 0.2μm is shown in Fig. 2(a), and flood ion beam implantation through a mask with a 0.2μm square hole is shown in Fig. 2(b). In the

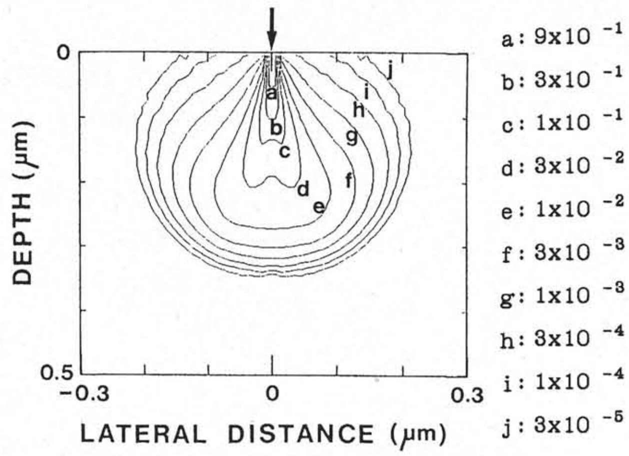


Fig. 1 Normalized two-dimensional equi-concentration contours of Frenkel pairs for an ion implanted point.

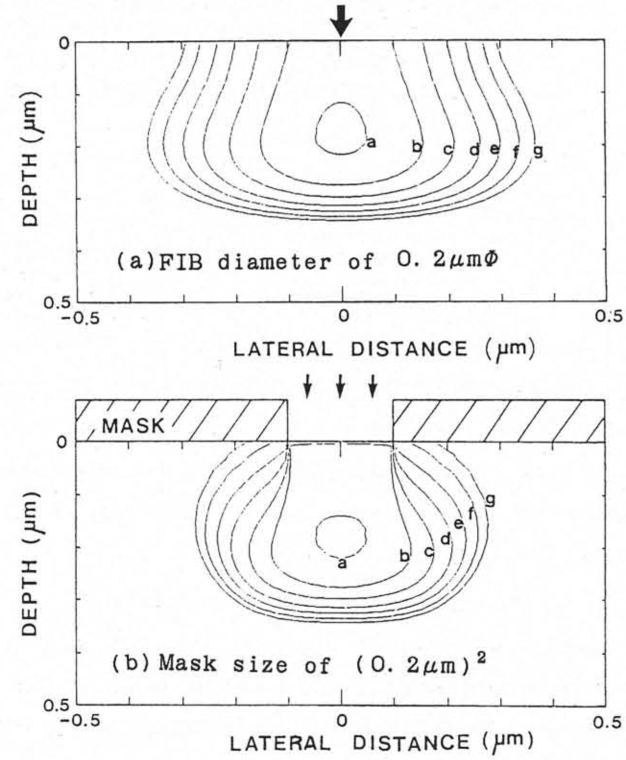
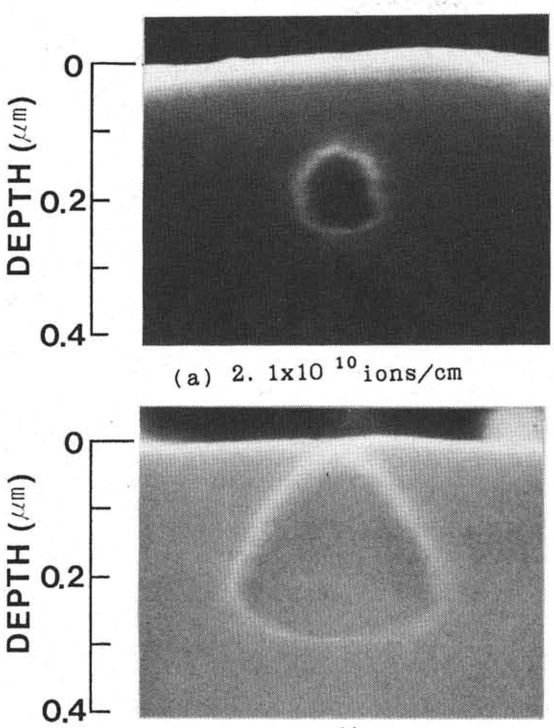


Fig. 2 Comparison of normalized two-dimensional Frenkel pair density contours.

peak concentration regions for both cases, the shapes of the Frenkel pair density profiles were almost the same. This result indicates that the fineness of the 70keV B^+ ion implanted layers tends to depends more on the lateral straggling of the ions than on the ion beam intensity profile.

B. Two-dimensional damage profile --- Cross sectional SEM micrographs of the line-scanned B^+ FIB implanted layers after Wright etching are shown in Fig. 3. Antimony doped 0.003 Ω cm Si substrates were used. At a low line dose, the etched regions remained under the surface. With an increase in the line dose, the etched hole became larger, its contour shape changed. Through comparison with the TEM micrograph in Fig. 4, it is confirmed that these etched regions correspond to the completely amorphous region [6].

The shapes of the etched contours provide good agreement with those of the simulations shown in Fig. 2, except in the surface region. This discrepancy might be due to the annealing out of defects in the surface region during implantation.



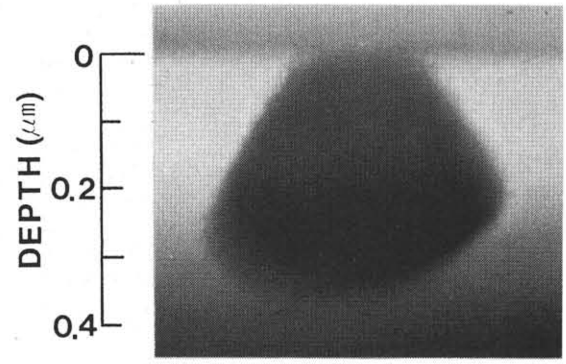
(a) 2. 1x10 ^{10} ions/cm

(b) 1. 1x10 ^{11} ions/cm

Fig. 3 Cross sectional SEM micrographs of line-scanned B^+ FIB implanted layers.

C. Mask-size dependence of profiles --- Monte Carlo simulation was employed to predict the mask size dependence of the damage profiles in the ion implanted submicron region. The dependence of depth on mask size is shown in Fig. 5. This depth is for the maximum Frenkel pair concentration normalized by the depth of the maximum boron concentration, R_{Fmax}/R_{Nmax}. The results indicate that the normalized maximum Frenkel pair depth moves toward the surface with a decrease in the mask size to below the threshold size, except in the case of As^+ ion implantation. This mask size effect is attributed to the lateral straggling of ions implanted into the Si. For heavy ions, the knock-on effect is more dominant in terms of damage accumulation. Thus, the damage profiles should be deeper than the simulated results.

With the reduction in mask size, it was predicted that the two-dimensional damage profile becomes would come to be more dependent on the mask size. This mask size effect should play an important role in secondary defect growth.



1. 4x10 ^{11} ions/cm

Fig. 4 Cross sectional TEM micrograph of line-scanned B^+ FIB implanted layers.

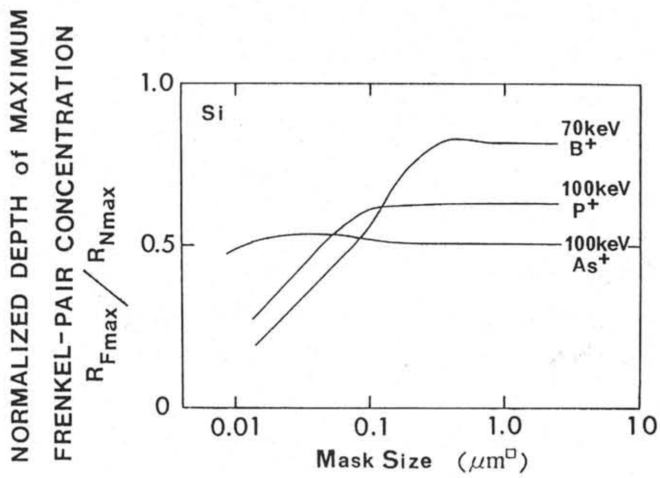


Fig. 5 Dependence of normalized depth for maximum Frenkel pair concentration on mask size.

D. Secondary defect profiles --- TEM micrographs of the B^+ FIB implanted Si layers after annealing at 800 and 1000°C for 15min are compared in Fig. 6. The line doses were $2x10^{10}$ and $1x10^{11}$ ions/cm. Two significant features can be seen in the figure.

First, when the amorphous region did not remain in the as-implanted layer, the residual secondary defects after annealing were larger and deeper as well for 1000°C annealing than those for when the amorphous region did remain. In particular, a large dislocation loop grew along the <111> direction after 1000°C annealing. This is believed to be influenced by the effect of a statistical variation in the defect growth that is caused by the damaged region in the as-implanted layer having small dimensions.

Second, when the amorphous layer remained, the dislocation loops continued to exist at about 0.2μm below the surface after the 800°C annealing. These loops stayed in the same general area but grew larger after 1000°C annealing. These types of secondary defect formation in the two-dimensionally limited small region should be investigated more in relation to the impurity diffusion profile.

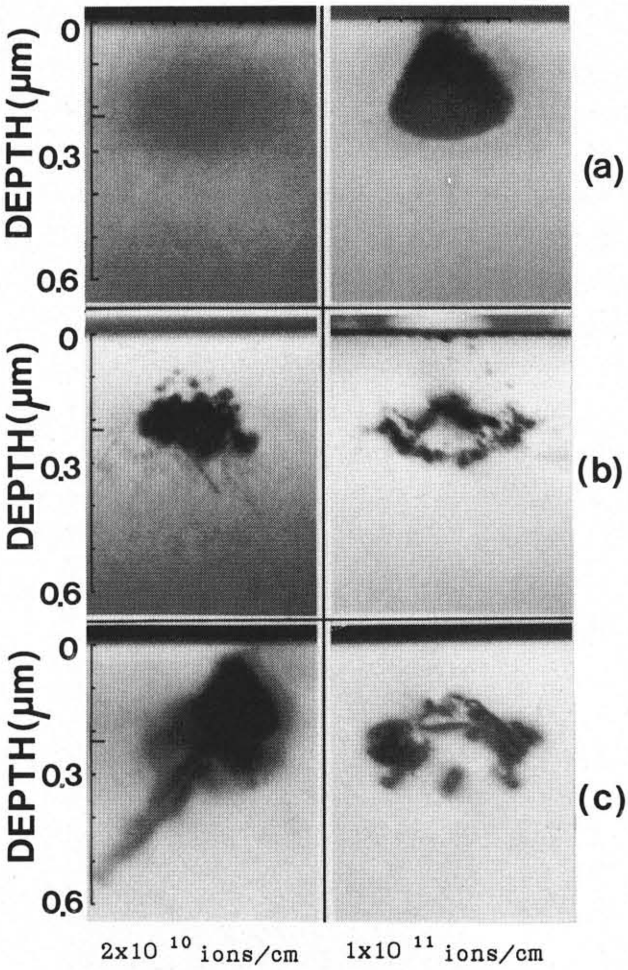


Fig. 6 Cross sectional TEM micrographs of secondary defect in B^+ FIB implanted layers after annealing. (a)as-implanted, (b)800°C annealed, (c)1000°C annealed.

5. Conclusion

The two-dimensional distribution of damage was calculated using a Monte Carlo program with the Kinchin-Pease equation for ion implantation into submicron areas of Si. The simulated results predicted that the damage profiles have strong mask size dependences. This is considered to play an important rûle in the secondary defect growth. The two-dimensional distribution of damage and secondary defects in B^+ FIB implanted Si layers was evaluated by using cross sectional SEM and TEM observations. The experimental results on the damage profiles provided qualitative agreement with those of the simulations.

6. References

[1]T. Ishitani, A. Shimase and S. Hosaka; Jpn. J. Appl. Phys., 22, p329, 1983.
[2]G. Moliere; Z. Nat., A2, p133, 1947.
[3]G. H. Kinchin and R. S. Pease; Rep. Prog. Phys., 18, p1, 1955.
[4]M. W. Jenkins; J. ECS, 124(5), p757, 1977.
[5]J. Albers; IEEE ED-32, p1930, 1985.
[6]J. Fletcher, et al.; Inst Phys. Conf. Ser., 60, p295, 1981.