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Effect of Energy Transport with Recoil Atoms on Deposited Energy Distribution in Silicon Irradiated with Energetic Ions

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Abstract: Contribution of recoil atoms to the spatial distribution of total energy deposited by ions impinging in silicon is evaluated for 10–250 keV B and Ar ions. The calculated results are compared with the damaged layer thickness obtained by the ion-bombardment-enhanced selective etching, and the effect of energy transport with recoil atoms (recoil atom effect) on deposited energy distributions is discussed.

Keywords: Energy transport, Deposited energy, Recoil atom, Damaged layer thickness

1. Introduction

Evaluation of spatial distribution of energy deposited by impinging ions in the target is necessary for understanding the irradiation-induced amorphization, because vacancy generation depends on the deposited energy.

The energy deposition mainly occurs in the primary knock-on process. Recently, we have performed a simplified evaluation of the distribution of deposited energy transfer rate on the basis of the extended LSS theory[1),2)], by considering only the primary knock-on process[3)]. The calculations were compared with the experimental results for lower energy (10–20 keV) ion-bombardment-enhanced selective etching (IBESE) of silicon, and a small discrepancy was observed between the calculations and the experimental damaged layer thickness in the dose region higher than 10^{15} ions/cm^2.

In this paper, first, we present the simplified evaluation for high incident energy (250 keV) Ar ions in Sec. 2. The calculations show a good agreement with the experimental results than those for the lower incident energy ions. Thus, it will be found that the simplified evaluation method gives a good estimation for high incident energy ions, though modification is necessary for lower incident energy ions. Second, we perform a more precise calculation in Sec. 3. The previous method is extended, considering the energy transport of recoiled target atoms, and the deposited energy distributions are presented for B and Ar ions with various incident energy conditions. The results of the calculation are compared with the experimental data, and contribution of the recoil atoms to the total deposited energy will be discussed.

2. Simplified Evaluation for High Energy Ion

Previously, we have presented the simplified evaluation of deposited energy distribution by utilizing the extended LSS theory[3)]. In the calculation, only the primary knock-on process is considered. The incident ion transfers its energy into electronic excitation and nuclear collision processes and stops at a certain depth in the target. The nuclear process consists of the displacement collision and the lattice site atom vibration. The ion-induced amorphization of crystals is closely related to the energy transfer rate into the atomic displacement. If we express the average depth, at which the j-th displacement collision occurs, as $\langle X_P(E_0, E^*)\rangle_j$ and the standard deviation of $\langle X_P\rangle$ as $\langle \Delta X_P^2(E_0, E^*)\rangle_j$, then the distribution of the energy transferred into the displacement process for the j-th collision is approximated by the Gaussian distribution,

$$F_j(X_P) = \frac{\langle T_d\rangle_j}{\sqrt{2\pi\langle \Delta X_P^2(E_0,E^*)\rangle_j}} \times \exp\left(-\frac{\left(X_P - \langle X_P(E_0,E^*)\rangle_j\right)^2}{2\langle \Delta X_P^2(E_0,E^*)\rangle_j}\right), \quad (1)$$

where E_0 is the initial ion energy, E^* the instantaneous ion energy after the j-th displacement, and $\langle T_d\rangle_j$ the averaged transferred energy in the j-th displacement collision. Thus, the total energy trans-

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fer rate at the depth X_P can be obtained by

$$\left(\frac{dE_{nd1}}{dX_P}\right)_{X_P} = \sum_{j=1}^{n} F_j(X_P), \qquad (2)$$

where n is the number of displaced atoms created in the primary knock-on process. For the total dose N_D, the density of energy deposited by ions at the depth X_P in the primary process is expressed as

$$E_{D1} = \left(\frac{dE_{nd1}}{dX_P}\right)_{X_P} N_D. \qquad (3)$$

In **Figs. 1(a)** and **1(b)**, dose dependence of damaged layer thickness is shown for the irradiation of 10 (△), 20 (○), and 250 (●) keV Ar ions. The solid lines show the depth where the deposited energy E_{D1} equals to 0.05 eV/Å^3(**Fig. 1(a)**) and 0.25 eV/Å^3(**Fig. 1(b)**). The experimental thickness of the damaged layer was estimated by using the ion-bombardment-enhanced selective etching (IBESE)[4].

For 250 keV irradiation shown in **Fig. 1(b)**, the experimental results show a good agreement with the depth of E_{D1}=0.25 eV/Å^3. By contrast, for low energy irradiation shown in **Fig. 1(a)**, a small discrepancy is observed between the experimental results and the calculations especially in the higher dose region, and the damaged layer thickness is slightly larger than the depth of E_{D1}=0.05 eV/Å^3. Thus, we can conclude that the simplified evaluation method gives a reasonable estimation for high incident energy ions, but it needs to be improved for the low incident energy ions. For more precise calculation, the effect of energy transport with recoil atoms (recoil atom effect) should be taken into consideration.

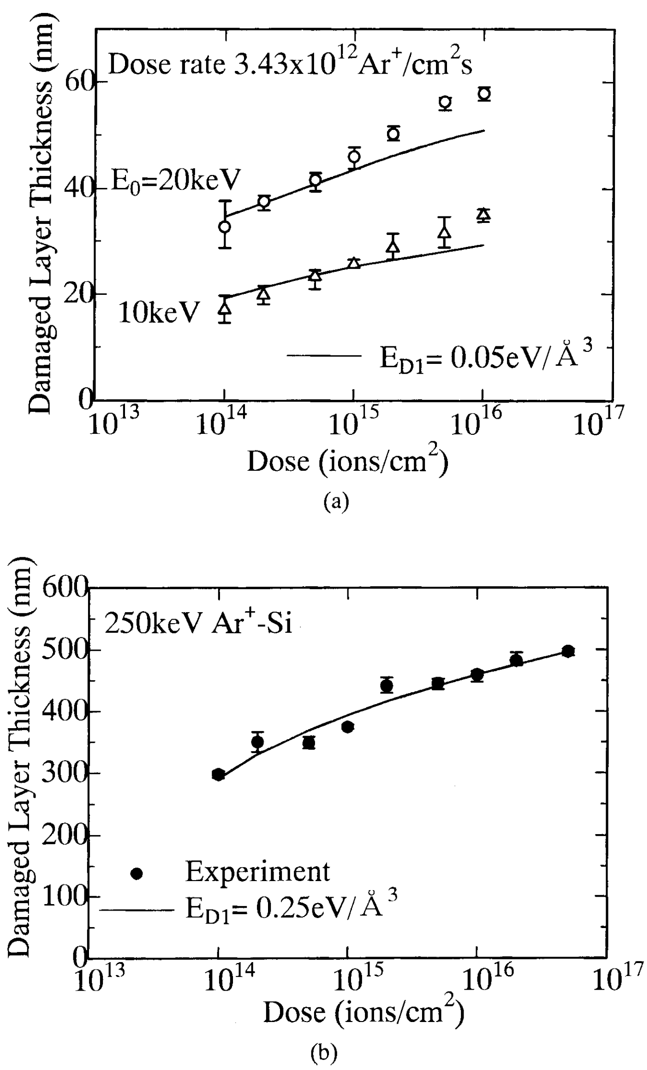

Fig.1 Dose dependence of damaged layer thickness for irradiation of (a) 10 keV (△) and 20 keV (○) Ar ions, and (b) 250 keV (●) Ar ions. The solid lines show the depth where deposited energy E_{D1} equals to (a) 0.05 and (b) 0.25 eV/Å^3.

3. Effect of Energy Transport with Recoil Atoms

3.1 Brice method

We develop the damage evaluation method to include the recoil atom effect on the basis of the method[5] proposed by Brice. According to the Brice's method, the spatial moments of the distribution of energy deposited into atomic processes are related to the average projected range of a primary recoil atom in two ways (RET1 and RET2), where RET stands for recoil energy transport.

In the RET1 method, it is assumed that the primary recoil atoms deposit their energy uniformly along a straight line from the target location where they were initially set in motion to the point where they stopped. It is also assumed that the primary recoil atoms travel parallel to the incident direction of the injected ion. If $R_{rp}(E_{rj})$ represents the average projected range of a primary recoil atom with initial energy E_{rj} for the j-th displacement collision, and $\Delta R_{rp}(E_{rj})$ represents the standard deviation in the parallel direction, then the assumption of uniform energy deposition rate yields

$$m(E_{rj}) = 1/2R_{rp}(E_{rj}), \qquad (4)$$

$$\sigma^2(E_{rj}) = 1/12R_{rp}^2(E_{rj}) + \left(\Delta R_{rp}(E_{rj})\right)^2, \qquad (5)$$

where m and σ^2 are the first and the second spatial moments of the depth distribution of energy deposited by total recoil atoms, respectively.

In the RET2 method, the moments of the deposited energy distribution by the total recoil atoms are related to the moments of the range distribution of the primary recoil atoms, assuming that most of recoil atoms have low kinetic energy, and at low energy the ratio of the central moments of the energy and range distributions are approximately constant[6]. Calculations suggest that the average damage depth due to the primary recoil atoms should be taken as 0.8 times the projected range, and also the standard deviation of the recoil atom damage distribution in the parallel directions should be taken as 0.8 times the corresponding value for the recoil atom range distribution[6]. Thus, m and σ^2 can be expressed as

$$m(E_{rj}) = 0.8R_{rp}(E_{rj}), \tag{6}$$

$$\sigma^2(E_{rj}) = 0.8\big(\Delta R_{rp}(E_{rj})\big)^2. \tag{7}$$

In a displacement collision, the target atoms gain the effective binding energy U_d, and the total energy transfer rate at a penetration depth X_P can be obtained by

$$\left(\frac{dE_{nd1}}{dX_P}\right)_{X_P} = \sum_{j=1}^{n}\big(F_{0j}(X_P) + F_{rj}(X_P)\big), \tag{8}$$

where

$$F_{0j}(X_P) = \frac{U_d}{\sqrt{2\pi\langle\Delta X_P^2(E_0,E^*)\rangle_j}} \times \exp\left(-\frac{\big(X_P - \langle X_P(E_0,E^*)\rangle_j\big)^2}{2\langle\Delta X_P^2(E_0,E^*)\rangle_j}\right), \tag{9}$$

and

$$F_{rj}(X_P) = \frac{E_{rj}(X_P)}{\sqrt{2\pi\big(\langle\Delta X_P^2(E_0,E^*)\rangle_j + \sigma^2(E_{rj})\big)}} \times \exp\left(-\frac{\big(X_P - \langle X_P(E_0,E^*)\rangle_j - m(E_{rj})\big)^2}{2\big(\langle\Delta X_P^2(E_0,E^*)\rangle_j + \sigma^2(E_{rj})\big)}\right). \tag{10}$$

$F_{0j}(X_P)$ and $F_{rj}(X_P)$ are the distributions of energy transfer rate at a penetration depth X_P for the j-th displacement collision by the incident ion and the primary recoil atom, respectively. In the calculation, U_d was assumed to be 15.8 eV[7].

3.2 Results

By employing RET1 and RET2 methods, the energy transfer rate into atomic displacement was evaluated as a function of penetration depth. For comparison, evaluation was also performed with the simplified methods, in which only the primary knock-on process was considered. **Figure 2** shows the results for Ar ion irradiation with initial energy of 10, 20, and 250 keV. For the lower initial ion energy of 10 and 20 keV, distributions of the energy transfer rate evaluated with the Brice methods is different from that with the simplified method, particularly, in the shallow region, and the peak position for RET1 and RET2 is deeper than that for the simplified method. By contrast, for the higher initial ion energy of 250 keV, little difference is ob-

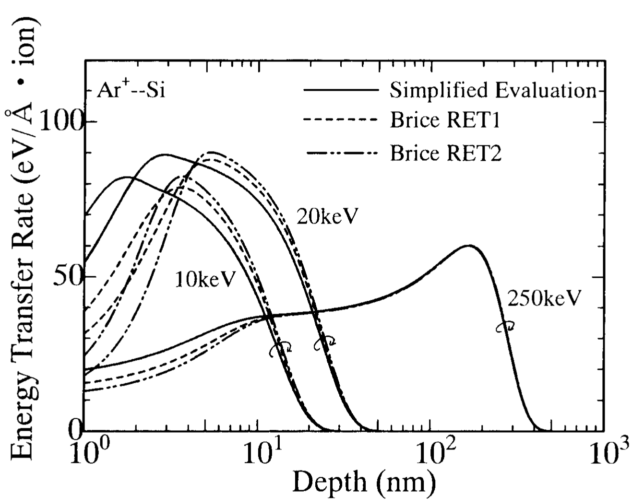

Fig.2 Distributions of energy transfer rate for Ar ions with initial energy of 10, 20 and 250 keV. They were calculated with the simplified evaluation, RET1, and RET2 methods.

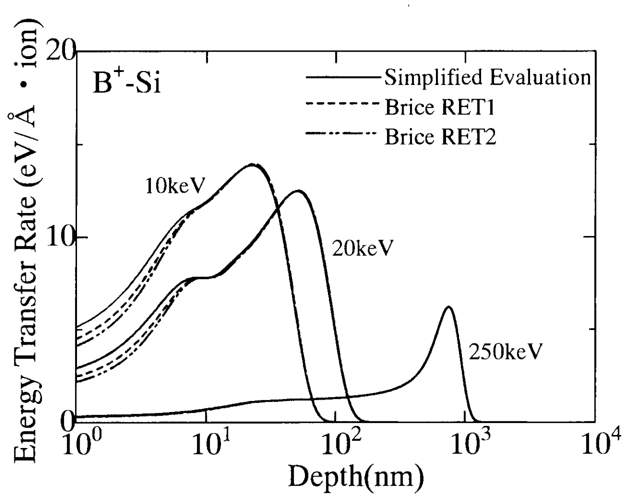

Fig.3 Distributions of energy transfer rate for B ions with initial energy of 10, 20 and 250 keV. They were calculated with the simplified evaluation, RET1, and RET2 methods.

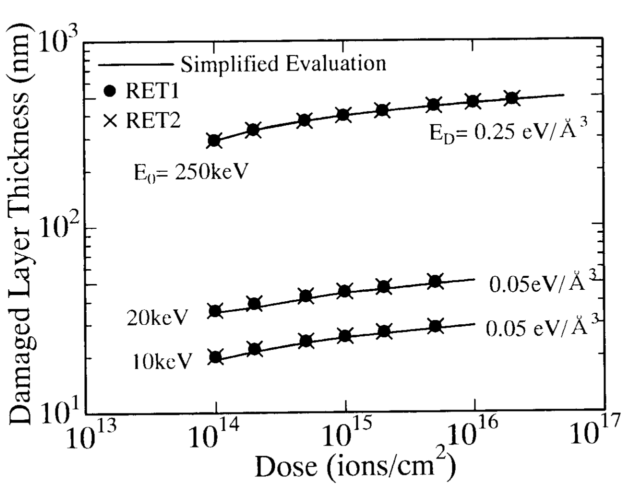

Fig.4 Damaged layer thickness evaluated by the simplified (solid curve), RET1 (●), and RET2 (×) methods. The thickness is assumed to correspond to the depth where the deposited energy E_D is a constant value.

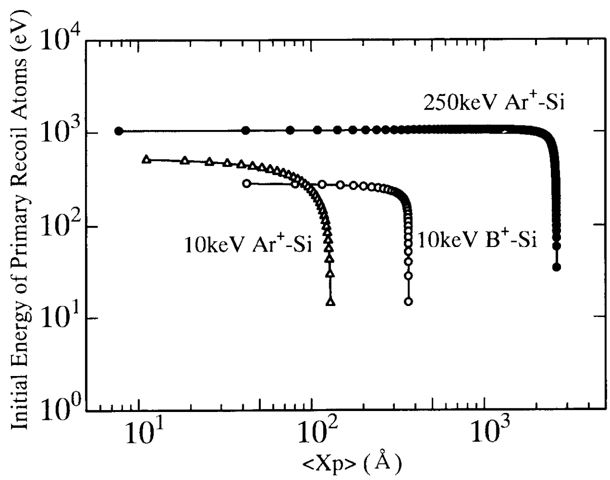

Fig.5 Initial energy of primary recoil atoms as a function of depth $\langle X_P \rangle$, at which they are produced, for irradiation of 10 (△) and 250 (●) keV Ar and 10 keV B (○) ions.

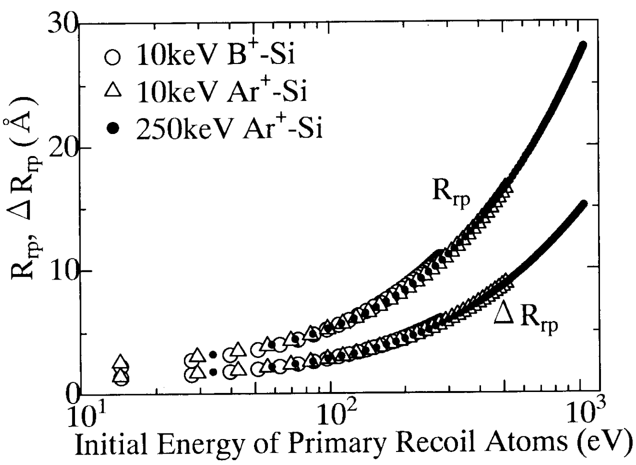

Fig.6 Average range R_{rp} of primary recoil atoms for 10 (△) and 250 (●) keV Ar and 10 keV B (○) ions and the standard deviation ΔR_{rp} as a function of the initial energy.

served among the distributions for the three methods, except for the small disagreement in the shallow region. Thus, it is found that the recoil atom effect is significant for the low energy ion irradiation.

The contribution of the recoil atoms can depend on the mass of the incident ions, thus we next examine the recoil atom effect for the lighter ions. **Figure 3** shows the results for B ions with incident energy of 10, 20, and 250 keV. For the case of B ions, the distributions calculated with the three methods show a better agreement with each other than those for Ar ions in all incident energy conditions, and the profiles have peaks at the same depth position. From **Figs. 2** and **3**, we can conclude that recoil atom effect on the distribution of energy transfer rate is larger for heavier ions and lower initial energy.

In **Fig. 2**, we must pay attention to another important feature, which is the tails of the curves. Slope of the tails is important in estimation of the damaged layer thickness. It is possible that the modification of the slope gives a better fit to the experimental data of the depth where the deposited energy equals to a constant value. The comparison among the depth calculated by the three methods is shown in **Fig. 4**. However, the calculated depth is almost the same for all methods, and a better agreement should not be expected between the depth and the experimental damaged layer thickness, in spite of the consideration of the recoil atom effect.

3.3 Discussion

The recoils deposit energy deeper in the target during the higher-order knock-on process, and the recoil atom effect can change the distribution of the energy transfer rate into atomic displacement. Thus, we investigate the range of primary recoil atoms and their standard deviation as a function of the depth where they are produced.

Figure 5 shows the initial energy of primary recoil atoms produced at the depth $\langle X_P \rangle$ for 10 and 250 keV Ar and 10 keV B ions. It is assumed that all recoils are silicon atoms. We can see that the initial

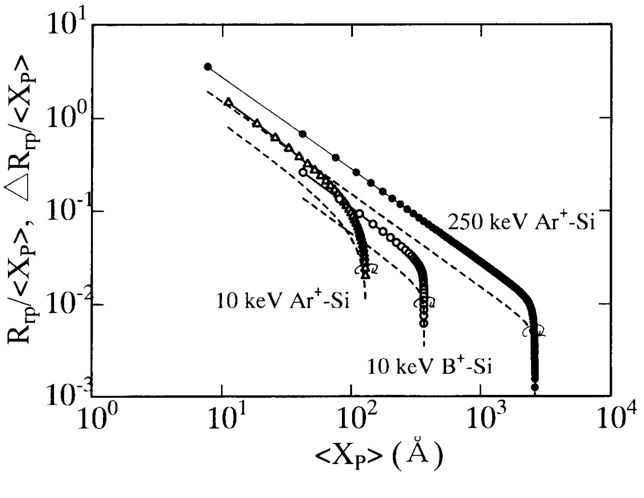

Fig.7 Average range R_{rp} and the standard deviation ΔR_{rp} of primary recoil atoms as a function of depth $\langle X_P \rangle$, where they are produced. The ordinate is normalized by $\langle X_P \rangle$.

energy of primary recoil atoms is much smaller than the initial energy of incident ion and hardly depends on the depth where they are produced, except for the tail of a displacement collision cascade.

Figure 6 shows dependence of the average projected range R_{rp} and its standard deviation ΔR_{rp} on the initial energy of primary recoil atoms for 10 and 250 keV Ar and 10 keV B ions. It can be seen that the R_{rp} and the ΔR_{rp} are much smaller than the depth $\langle X_P \rangle$, where the primary recoils are produced, shown in **Fig. 5**, and they decrease with decreasing the initial energy of primary recoils.

From **Figs. 5** and **6**, we have estimated ratio of the range R_{rp} of primary recoil atoms and their standard deviation ΔR_{rp} to the depth $\langle X_P \rangle$, where they are produced, as a function of $\langle X_P \rangle$. The results are shown in **Fig. 7**. From **Fig. 7**, we can see that $R_{rp}/\langle X_P \rangle$ and $\Delta R_{rp}/\langle X_P \rangle$ are large in the shallow region, and they monotonically decrease with increasing $\langle X_P \rangle$. Furthermore, in the last stages of a displacement collision cascade, they drastically decrease. Therefore, the modification of the energy transfer rate by the recoil atoms is significant only near the surface, as shown in **Figs. 2** and **3**, because the initial energy of primary recoil atoms is large in the surface region.

However, initial energy of the recoils is much smaller than the instantaneous energy of the incident ion, and the range of the recoils is also very small. Thus, the contribution of recoil atoms to the total deposited energy is negligible in deeper region, and the recoil atom effect is insufficient for the explanation of the dose dependence of the damaged layer thickness obtained by the IBESE for low energy Ar ions. For more precise calculation, it may be necessary to consider the effects of channeling, annealing, and ion dose rate.

4. Conclusion

The effect of energy transport with recoil atoms has been investigated for Ar and B ion irradiation in silicon. It has been shown that damaged layers caused by high energy (250 keV) ion irradiation can be evaluated correctly by the simplified evaluation method, considering only the primary knock-on process. In order to extent the applicability of the evaluation method to the lower energy region of 10–20 keV, the recoil atom effect has been estimated. From the calculations, it has been shown that the effect is significant for heavier and lower incident energy ions, particularly in the shallow region. However, the recoils less affect the total deposited energy distributions, and the modification did not improve the fit of the experimental data to the calculations. For more reasonable evaluation of damage induced by the low energy ions, it should be necessary to consider the effects of channeling, annealing, and ion dose rate.

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