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https://doi.org/10.15017/1485033

出版情報：九州大学大学院システム情報科学紀要. 2 (1), pp.59-64, 1997-03-26. Faculty of Information Science and Electrical Engineering, Kyushu University
バージョン：
権利関係：

九州大学大学院
システム情報科学研究科報告
第2巻 第1号 平成9年3月

Research Reports on Information Science and
Electrical Engineering of Kyushu University
Vol.2, No.1, March 1997

Simplified Evaluation of Displacement Effect Distribution in Silicon Irradiated with Low-Energy Ions

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(Received December 24, 1996)

Abstract: Displacement effects induced by low-energy ion irradiation in silicon have been investigated theoretically. Instantaneous energy of an incident ion during its slowing-down process has been obtained as a function of the penetration depth and the ordinal number of displacement collisions by solving a set of integral equations. From these results, the averaged penetration depth as a function of the ordinal number of displacement collisions is estimated. The mean free path of the incident ion at a specific depth in silicon is also estimated for several initial energy values and ion species. The energy transfer rate into atomic displacement collisions and the density of deposited energy in a collision cascade have been evaluated considering the primary knock-on process. The damaged layer thickness obtained by the experiment of the ion-bombardment-enhanced selective etching of silicon crystals shows a good agreement with the depth where the estimated density of deposited energy takes a constant value.

Keywords: Low-energy ions, Displacement effect, Energy transfer rate, Deposited energy, Damaged layer thickness

1. Introduction

As the ULSI processing technology advances, the energy of ions utilized in the process becomes lower to fabricate very fine structures precisely. Energetic ions deposit their energy to the target atom nuclei and electrons during the stopping process. The dominant energy loss process in solids for low-energy ions is the nuclear stopping, while for medium or high energy ions, the electronic stopping matches with the nuclear stopping. Thus the effects induced by the irradiation of low-energy ions can be different from that of higher energy ions, and the understanding of irradiation-induced effects by low-energy ions in solids is becoming important.

Theoretical evaluation of behaviors of energetic particles in solids has been studied by many researchers. The methods are classified in two categories, i.e., Monte Carlo methods[1)] and integral equation methods[2)]. The most comprehensive theory for the integral equation is the LSS theory derived by Lindhard, Scharff, and Schiott[2)]. They have assumed a screened Coulomb potential (Thomas-Fermi potential) as the interaction potential of nuclear collisions and predicted the values of electronic energy loss and nuclear energy loss for many ion-target pairs. The range of ions in the target material can be obtained by solving the integral equations.

Recently, we have evaluated the damage function for low-energy ion irradiation[3)]. In the calculation we have divided the nuclear energy loss process into the displacement collision process and the excitation process of the lattice site atom vibration, and the results for the Si-Si collision agreed well with the experimental results of the pulse-height defect.

In this paper, we have first calculated the averaged value of instantaneous ion energy as a function of the penetration depth and that of the ordinal number of displacement collisions by utilizing extended LSS theory[4)]. From these results, the penetration depth has been estimated as a function of the ordinal number of displacement collisions in a collision cascade for several low-energy incident ions, and the trend of the mean free path for those ions is discussed. Next, we have evaluated the energy transfer rate and the deposited energy density of the incident ion for several initial energy values and ion species in the low-energy region (5–40 keV).

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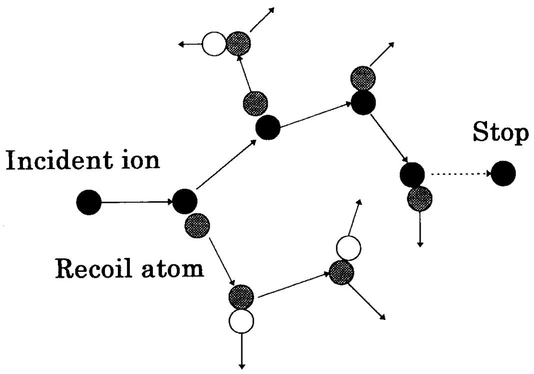

Fig.1 Schematic diagram of a collision cascade.

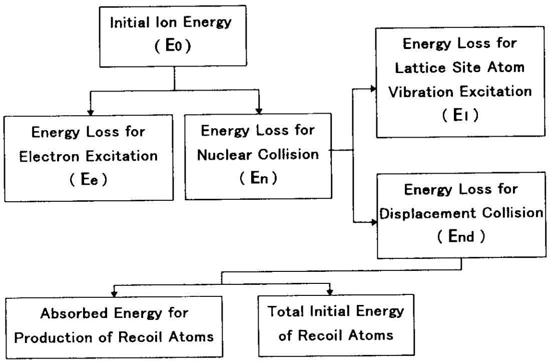

Fig.2 Energy partition relation in a collision cascade.

The calculated values are compared with the experimental results, and the amorphization of silicon is discussed. In the calculation, we have considered only the primary knock-on process and neglected the higher order knock-on, but the results show a relatively good agreement with the experimental results of the damaged layer thickness measurement.

2. Theory

The schematic diagram of a collision cascade is depicted in **Fig. 1**, where solid circles show the incident ion, hatched circles the primary knock-on atoms, and open circles the secondary or higher order knock-on atoms. For the simplicity of estimating first order effects, we have considered only the primary knock-on process in the present calculation.

The incident ion transfers its energy into electronic excitation and nuclear collision processes and stops at a certain depth in the target. The nuclear collision consists of the displacement collision and the lattice site atom vibration processes[5]. The energy partition relation for each process in a collision cascade is shown in **Fig. 2**. The amorphization of crystalline materials induced by ion irradiation is closely related to the energy transfer rate into atomic displacements in the collision. The energy transfer rate into atomic displacements at a penetration depth X_P is expressed as,

$$\left(\frac{dE_{nd1}}{dX_P}\right)_{X_P}, \tag{1}$$

where E_{nd1} is the energy loss for displacement collision, where the suffix 1 in E_{nd1} denotes the primary knock-on process[4]. For the total ion dose of N_D, the density of energy deposited by the impinging ions at the depth X_P in the primary process can be expressed as,

$$E_{D1} = \left(\frac{dE_{nd1}}{dX_P}\right)_{X_P} N_D. \tag{2}$$

The generalized equation for irradiation effects in the collision process is described as,

$$\frac{\partial\overline{\Phi}(E,X)}{\partial E} = \frac{-1}{N\big(S_e(E)+S_n(E)\big)}\frac{\partial\overline{\Phi}(E,X)}{\partial X}, \tag{3}$$

where $\overline{\Phi}(E,X)$, N, $S_e(E)$, and $S_n(E)$ are expected irradiation effect induced by an ion, density of the target, electronic, and nuclear stopping power, respectively, and E and X, the energy and the path length of the ion, respectively[4]. The formulae for $S_e(E)$ and $S_n(E)$ are presented by Lindhard et.al[2),6)]. From Eq. (3), the energy loss for each process shown in **Fig. 2** can be expressed as,

$$\frac{dE_e}{dX} = NS_e(E), \tag{4}$$

$$\frac{dE_n}{dX} = NS_n(E), \tag{5}$$

$$\frac{dE_{nd}}{dX} = NS_{nd}(E, E_d), \tag{6}$$

$$\frac{dE_l}{dX} = N\big(S_n(E) - S_{nd}(E)\big), \tag{7}$$

where E_d is the threshold energy for atomic displacement. Thus the average transferred energy in the j-th displacement collision, lattice site atom vibration, and electronic excitation processes are given by,

$$\langle T_d\rangle_j = \int_{E_j}^{E_{j-1}} \frac{S_{nd}(E,E_d)}{S_e(E)+S_n(E)}dE, \tag{8}$$

$$\langle T_l\rangle_j = \int_{E_j}^{E_{j-1}} \frac{S_n(E)-S_{nd}(E,E_d)}{S_e(E)+S_n(E)}dE, \tag{9}$$

$$\langle T_e\rangle_j = \int_{E_j}^{E_{j-1}} \frac{S_e(E)}{S_e(E)+S_n(E)}dE, \tag{10}$$

respectively, where E_j is the energy of the incident ion after the j-th displacement collision process. The energy conservation relation for the series of collision should be described as,

$$E_{j-1} = E_j + \langle T_d\rangle_j + \langle T_l\rangle_j + \langle T_e\rangle_j. \tag{11}$$

It is clear from **Fig. 2** that if the initial ion energy E_{j-1} for j-th collision can be obtained, the energy partition relation and total number of recoil atoms in the j-th collision can be computed. Thus, by repeating the calculation until no recoil atoms are produced, the energy partition relation in the collision cascade induced by the incident ion can be evaluated.

The average penetration depth where the ion energy during its slowing-down process is an arbitrary value E^* can be estimated by the extended LSS theory[4], and it is expressed as,

$$\langle X_P(E_0,E^*)\rangle = \int_{E^*}^{E_0} \frac{dE}{NS_{tr}(E)} \times \exp \int_{E_0}^{E} \frac{dE}{\lambda_{tr}(E)NS_{tr}(E)}, \tag{12}$$

and the standard deviation of the statistical distribution of $X_P(E_0,E^*)$ is given by,

$$\langle \Delta X_P^2(E_0,E^*)\rangle = \frac{1}{3}\Big(2\langle X_r^2(E_0,E^*)\rangle + \langle X_c^2(E_0,E^*)\rangle\Big) - \langle X_P(E_0,E^*)\rangle^2, \tag{13}$$

where E_0 and E^* are the initial energy and the instantaneous energy of the incident ion, respectively, and $\lambda_{tr}(E)$, $S_{tr}(E)$, $\langle X_r^2(E_0,E^*)\rangle$, and $\langle X_c^2(E_0,E^*)\rangle$ are functions of energy defined in Ref. 4. The energy transferred into the displacement process at a penetration depth X_P for the j-th collision can be approximated by a Gaussian distribution function with the parameters above and expressed as,

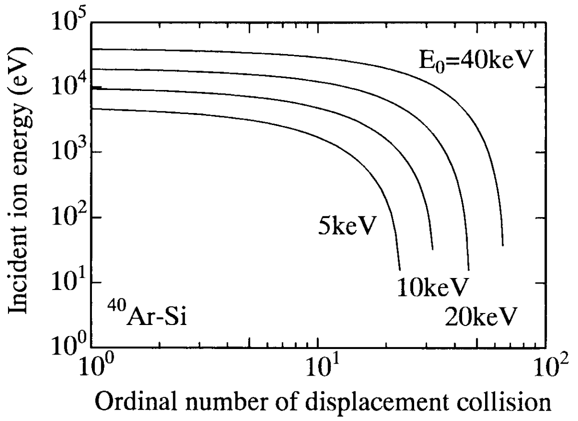

Fig.3 Ion energy as a function of the ordinal number of displacement collisions for Ar$^+$ with initial energy of 5, 10, 20, and 40 keV.

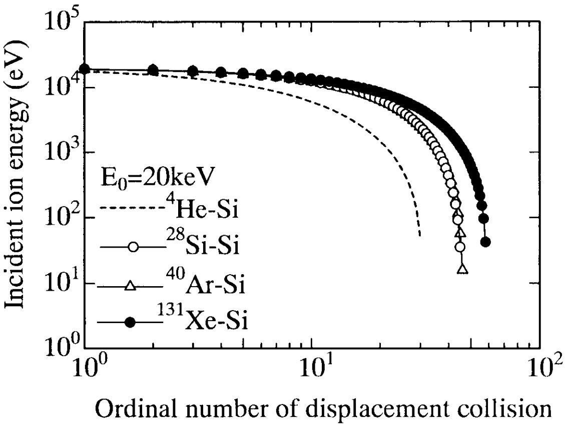

Fig.4 Ion energy as a function of the ordinal number of displacement collisions for He$^+$, Si$^+$, Ar$^+$, and Xe$^+$ with initial energy of 20 keV.

$$F_j(X_P) = \frac{\langle T_d\rangle_j}{\sqrt{2\pi\langle \Delta X_P^2(E_0,E^*)\rangle_j}} \times \exp\left(-\frac{\left(X_P-\langle X_P(E_0,E^*)\rangle_j\right)^2}{2\langle \Delta X_P^2(E_0,E^*)\rangle_j}\right). \tag{14}$$

Thus the total energy transfer rate at the depth X_P can be obtained by,

$$\left(\frac{dE_{nd1}}{dX_P}\right)_{X_P} = \sum_{j=1}^{n} F_j(X_P), \tag{15}$$

where n is the number of displaced atoms.

3. Results and Discussion

The ion energy after each displacement collision is calculated and shown in **Fig. 3** as a function of the ordinal number of the displacement collisions

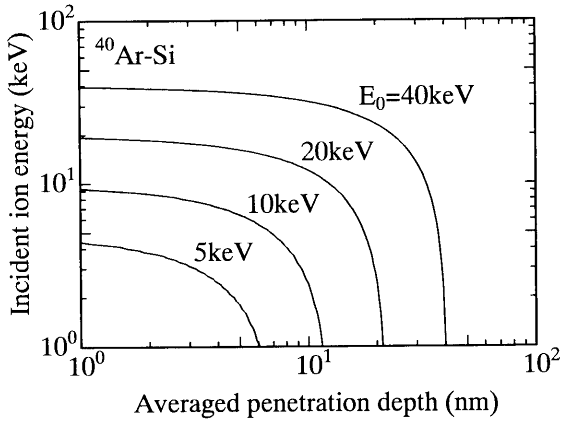

Fig.5 Ion energy as a function of penetration depth for Ar^+ with initial energy of 5, 10, 20, and 40 keV.

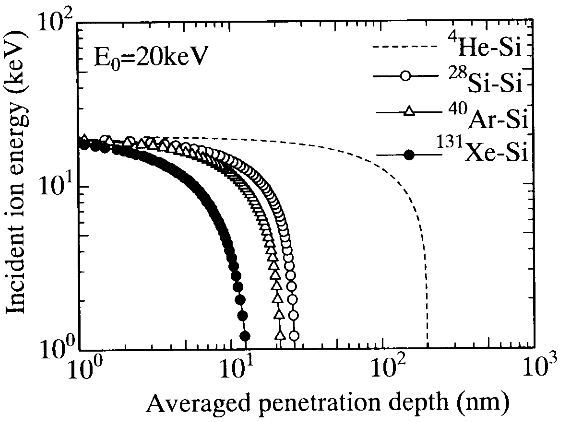

Fig.6 Ion energy as a function of penetration depth for He^+, Si^+, Ar^+, and Xe^+ with initial energy of 20 keV.

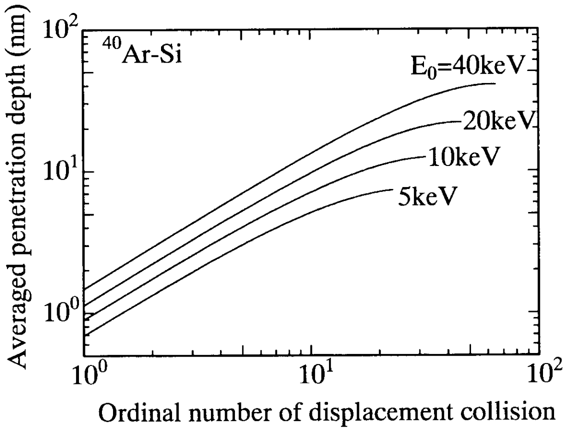

Fig.7 Penetration depth as a function of the ordinal number of displacement collisions for Ar^+ with initial energy of 5, 10, 20, and 40 keV.

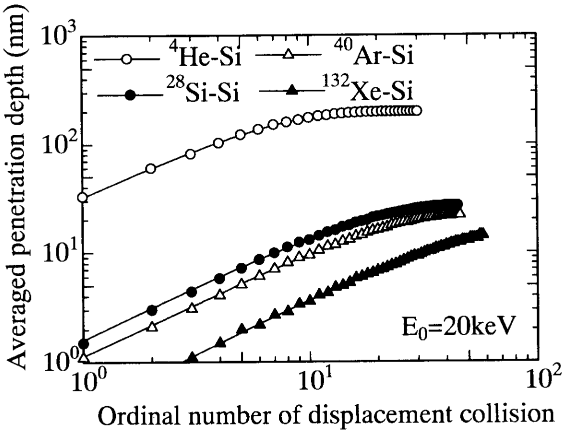

Fig.8 Penetration depth as a function of the ordinal number of displacement collisions for He^+, Si^+, Ar^+, and Xe^+ with initial energy of 20 keV.

for an argon ion with several different initial energy values. Similar calculation results for several ion species with the initial energy of 20 keV are shown in **Fig. 4**. In this initial energy region, the total number of displacement collisions increases remarkably with increasing the initial energy of the incident ion, and slightly depends on the ion species. The total number of the displacement collisions for a 20 keV silicon ion is almost the same as that for a 20 keV argon ion.

If we assume an instantaneous energy value of the incident ion during its slowing-down process in the target, we can calculate the corresponding value of the averaged penetration depth of the ion using Eq. (12). The results are shown in **Fig. 5** for argon ions with several different initial energy values. Similar calculation results for several ion species with the initial energy of 20 keV are shown in **Fig. 6**. It is found that the depth where the energy of the impinging ions reaches a specific value becomes deeper for higher initial energy and lighter particles.

By combining **Figs. 3** and **5** or **4** and **6**, we can obtain the penetration depth of incident ions as a function of the ordinal number of the displacement collisions. **Figures 7** and **8** show the depth for argon ions in silicon with different initial energy and for several ions in silicon with the initial energy of 20 keV, respectively. From **Figs. 7** and **8**, we can evaluate the mean free path of ions between each adjacent displacement collision process. The curves shown in **Figs. 7** and **8** are approximately straight lines except for the penetration tails, and the mean free path is larger for lighter species and higher initial energy ions.

From Eq.(15), the energy transfer rate into atomic displacements can be obtained as a function of penetration depth, and the results are shown in

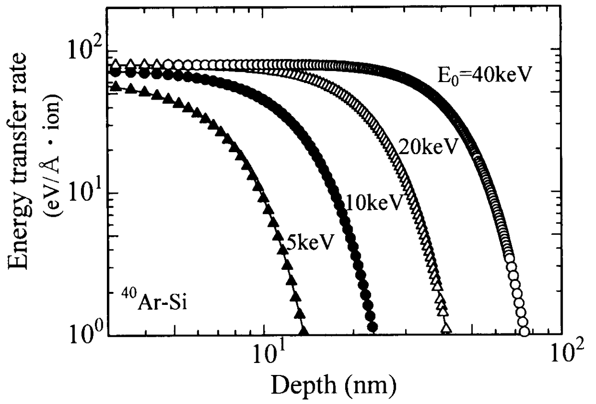

Fig.9 Energy transfer rate as a function of penetration depth for Ar^+ with initial energy of 5, 10, 20, and 40 keV.

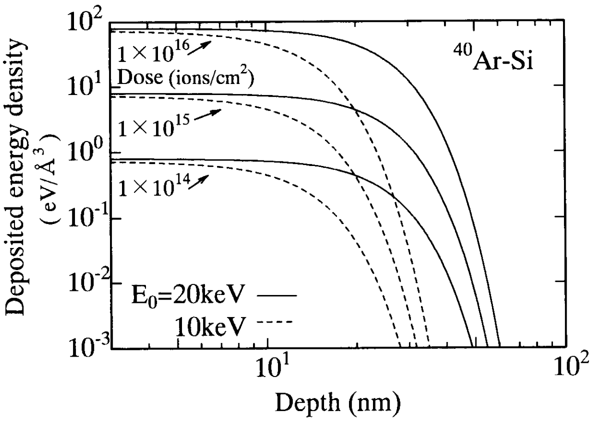

Fig.10 Density of deposited energy as a function of penetration depth for the irradiation of 10 and 20 keV Ar^+ to dose of 1×10^{14}, 1×10^{15}, and 1×10^{16} cm^{-2}.

Fig. 9 for an argon ion penetrating into silicon with various initial energy. It is found that the depth where the energy transfer rate reaches a specified value becomes deeper for higher initial ion energy.

Figure 10 shows the density of deposited energy in the primary process calculated by Eq. (2) for 10 keV and 20 keV argon ions in silicon with several dose values.

The density of deposited energy necessary for defining the damaged regions can be estimated from the curves shown in **Fig. 10** and the experimental data of the damaged layer thickness. Some examples of the experimental data of the damaged layer thickness[7)] are shown as a function of dose in **Fig. 11**, which were obtained by the ion-bombardment-enhanced selective etching (IBESE)[8)].

The open triangles and circles in **Fig. 11** show the damaged layer thickness for 10 keV and 20 keV argon ion irradiation, and the solid lines show the depth at which the density of deposited energy E_{D1} equals to 0.05 eV/Å^3 obtained from **Fig. 10**. The experimental results show a good agreement with the depth of $E_{D1} = 0.05$ eV/Å^3 in the dose region lower than $\sim 10^{15}$ ions/cm^2, while in the higher dose region, the damaged layer thickness is slightly larger than the depth of $E_{D1} = 0.05$ eV/Å^3. We speculate that the discrepancy between the experimental results and the calculated values in the higher dose region should be due to the underestimation of the density of deposited energy caused by neglecting the higher order knock-on processes. For more precise calculation, in which the effects by the secondary or higher order knock-ons are taken into account, the position of $E_{D1} = 0.05$ eV/Å^3 should shift deeper, especially at higher dose region.

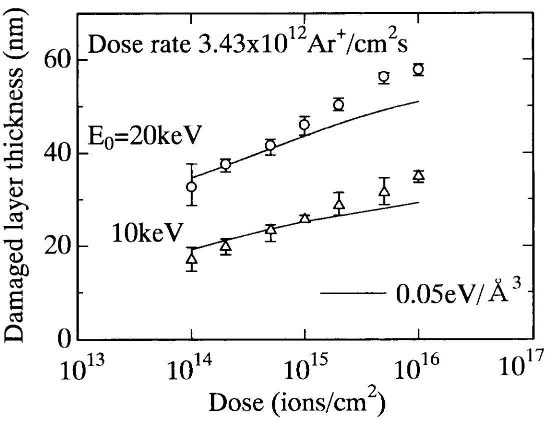

Fig.11 Dose dependence of damaged layer thickness for irradiation of 10(△) and 20 keV(○) Ar^+. The solid lines show the depth where deposited energy $E_{D1} = 0.05$ eV/Å^3.

Except for the small disagreement, we can conclude that the thickness of the damaged layer corresponds to the depth at which the density of deposited energy is a constant value of approximately 0.05 eV/Å^3 under the present experimental conditions.

4. Conclusion

The irradiation effects of low-energy ions in silicon have been investigated theoretically. In the theoretical calculation, we have considered only the primary knock-on process.

The total of displacement collisions remarkably increases with increasing the incident ion energy and slightly depends on the ion species. The mean free path of ions at a penetration depth in the target is larger for higher initial energy and lighter particles.

The dose dependence of the depth at which the density of the deposited energy reaches a constant value shows a good first order agreement with that of the damaged layer thickness obtained by the ion-bombardment-enhanced selective etching. For more precise simulation, the secondary or higher knock-on processes should be considered.

Acknowledgments

The authors are grateful to H. Tanoue of the Electrotechnical Laboratory for the assistance in the simulation by the extended LSS theory.

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