Ion implantation phenomena by binary collision approximation

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In the November 2020 issue of Applied Physics, an article entitled "Analyzing Ion Implantation Phenomena with Old and New MARLOWE" was published, which introduced a brief explanation of the MARLOWE code and examples of its application to compound semiconductors (1). The physical background in that article was not treated in detail. So, this article will show what the MARLOWE code analyses ion implantation phenomena based on collision theory. This article will guide to better understanding the phenomenon of ion implantation and to consider implantation in new materials.

Collision cascade

At first, what kind of collision phenomenon occurs when an ion hits the target is explained. Let the energy of the incident ion be E_0 and the atomic number be Z_1. Let the atomic number of the target be Z_2. When the incident ion collides with the target atom, the target atom is ejected from the lattice site when the energy is higher than the displacement energy E_d. Assuming that the energy of the incident ion after collision is E_1 and the energy of the ejected atom is E_2, the following cases can be classified.

$E_1>E_d$ $E_2>E_d$ ：vacancy production
$E_1<E_d$ $E_2>E_d$ $Z_1=Z_2$：replacement
$E_1<E_d$ $E_2<E_d$ $Z_1\neq Z_2$：Interstitial atom Z_1

The incident particle loses the energy and change direction as a result of collision with the nucleus. Until the next collision, the incident particle loses the energy through the collision with electrons. It will stop when the energy finally falls below the rest energy. The maximum energy received by the target atom is as follows.

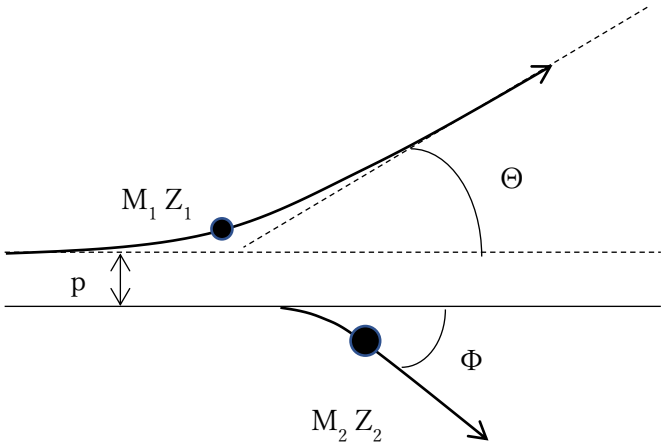
$$E_{max} = \frac{4M_1M_2}{(M_1+M_2)^2}E_0$$

For example, in the case of silicon, if boron is incident with energy of 100 keV, silicon will receive energy of 80 keV. Since this value is much larger than the displacement energy, a chain of displacements occurs one after another, forming a cascade. In this phenomenon, the pair of vacancies and interstitial atoms is called the Frenkel pair.

Two-body collision approximation

As shown in the figure below, consider the case where incident particles flying from infinity interact with a stationary target atom with energy E0 and collision coefficient p. It is assumed that the central force due to the two-body potential V (r) acts between the particles. The V(r) is determined by the relative distance(r)

between the two particles.



The energy transferred from the incident particle to the target atom can be expressed by the following

$$\Delta E = E_0 \frac{4M_1M_2}{(M_1+M_2)^2} sin^2 \frac{\Theta}{2}$$

formula.

The Θ is the scattering angle, assuming a spherically symmetric potential, the scattering angle is expressed by the following integral.

$$\Theta(p, E_c) = \pi - 2p \int_{r_{min}}^{\infty} \frac{dr}{r^2 \sqrt{1 - \frac{V(r)}{E_c} - \frac{p^2}{r^2}}}$$

In this equation, p is the impact parameter and Ec is the energy of the center of mass system.

$$E_c = E_0 \frac{M_2}{M_1 + M_2}$$

From the above, the energy loss due to the nucleus can be obtained by integrating the collision coefficient p as follows.

$$S_n(E) = 2\pi \int_0^{\infty} \Delta E(E,p) p dp$$

Inter-atomic potential

The scattering potential between the two positively charged nuclei is shielded by the electrons around the nuclei. The effect of the electron is expressed by the shielding function Φ (r).

$$V(r) = \frac{Z_1 Z_2 q^2}{4\pi\epsilon_0}\Phi(r)$$

Ziegler, Biersack, and Littmark analyzed the combination of 522 atoms and derived the universal screening potential (2). This ZBL potential is used in the field of ion implantation.

$$\Phi(x) = 0.1818e^{-3.2x} + 0.5099e^{0.9423x} + 0.2802e^{-0.4029x} + 0.02817e^{-0.2016x}$$

$$x = \frac{r}{a_U} \quad a_U = 0.8854\frac{a_0}{Z_1^{0.23}+Z_2^{0.23}}$$

The a_U is the screening distance and a_0 is the Bohr radius.

Electronic stopping

The energy loss due to electrons is a combination of Lindhard's LSS theory (3), which does not depend on the collision coefficient, and the Oen-Robinson model, which depends on the collision coefficient. In other words, it can be divided into non-local and local parts.

$$\Delta E = \Delta E_{nl} + \Delta E_{loc}$$

Non-local part is applicable for large collision coefficients, while Local part is associated with individual collisions. Non-local energy loss is expressed as follows (4).

$$\Delta E_{nl} = NS_e\Delta R\left[x_{nl} + x_{loc}\left(1 + \frac{p_{max}}{a}\right)exp\left(-\frac{p_{max}}{a}\right)\right]$$

Where ΔR is the distance the particles move before they collide, N is the number density of the target atom, Se is the electronic blocking cross section, and pmax is the maximum collision coefficient to which the local energy loss is applied. The contribution from the impact parameter larger than this will be treated in this equation. On the other hand, the Local energy loss is as follows (4).

$$\Delta E_{loc} = x_{loc}\frac{S_e}{2\pi a^2}exp\left(-\frac{R(p,E)}{a}\right)$$

$$a = \frac{a_U}{\gamma}$$

$$S_e = k_{corr}k\sqrt{E}$$

Here, γ is a parameter for associating with the experimental results. Se is an energy loss based on the LSS theory by Lindhard, et al.

The kcorr is a parameter to correspond to the experimental result, and k is expressed as follows (3).

$$k = 8\pi h a_0 \sqrt{2} \frac{Z_1^{\frac{7}{6}} Z_2}{\left(Z_1^{\frac{2}{3}} + Z_2^{\frac{2}{3}}\right)^{\frac{3}{2}} \sqrt{M_1}}$$

The ratio of non-local to local part is expressed by the following formula.

$$x_{nl} + x_{loc} = 1$$

In the case of silicon, the value can be determined by the following relational expression from many experimental data (5).

$$x_{nl} = y_{nl} E^q$$

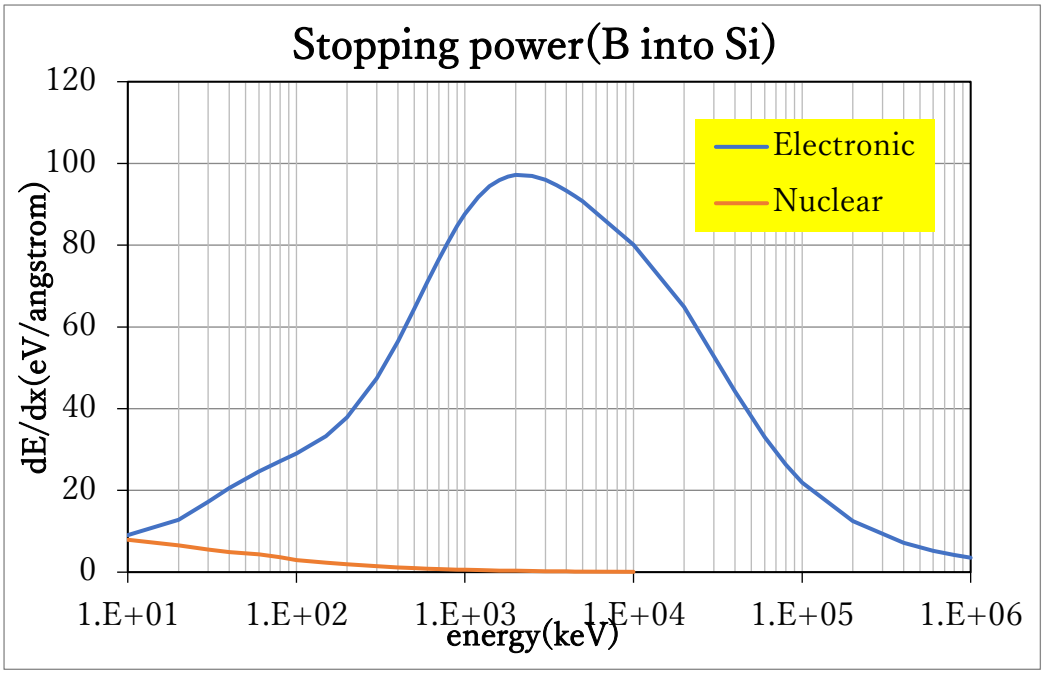
For example, when injecting boron into silicon, the following values are proposed.

$k_{corr} = 1.75$
$a_U = 0.45$
$y_{nl} = 0.05$
$q = 0.23$

The energy loss due to collision is expressed as the sum of the nuclear loss and the electronic loss described above.

$$\frac{dE}{dx} = -N[S_n(E) + S_e(E)]$$

It shows the general trend of energy dependence of nuclear energy loss and electronic energy loss.



If the energy is lower than the target valence electron velocity (Fermi velocity), the energy loss is proportional to the square root of the ion velocity.

Debye temperature

The lattice vibration of the target atom affects the orbit of the incident ion. When the substrate temperature rises, channeling is hindered by lattice vibration. The thermal vibration of lattice atoms is expressed by the following equation.

$$f(dx, dy, dz) = \frac{1}{\sqrt[3]{2\pi\sigma^2}} exp\left(-\frac{dx^2 + dy^2 + dz^2}{2\sigma^2}\right)$$

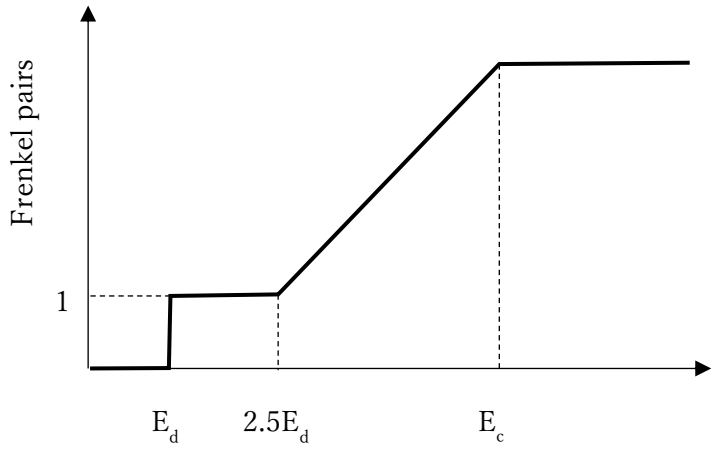
The standard deviation of atomic displacement from the rest position is obtained from Debye theory (6).

Damage

Frenkel pairs

The collision cascade displaces atoms from the lattice sites to form vacancies, and the displaced atoms become interstitial atoms. These are called Frenkel pairs. A Kinchin-Pease model was proposed to estimate the number of Frenkel pairs (7). In this model, the collision is assumed to be two-body scattering, and the displacement due to the collision with the nucleus does not occur at the energy Ec or higher. The number of Frenkel pairs is assumed to be a function of the energy given to the initial recoil atom (PKA) by the incident ion. This function is as follows.

$$Frenkel\ pairs = 0 \ \ for\ 0 < T < E_d$$
$$Frenkel\ pairs = 1 \ \ for\ E_d < T < 2E_d$$
$$Frenkel\ pairs = \frac{T}{2E_d} \ \ for\ 2E_d < T < E_c$$
$$Frenkel\ pairs = \frac{E_c}{2E_d} \ \ for\ T > E_c$$



Energy of Primary Knock-on Atom

The above Ec is the boundary value between nuclear energy loss and electronic energy loss. The nuclear energy loss is dominant in the energy region less than Ec. The electronic energy loss os dominant in the energy region larger than Ec.

References

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