# Issues of the analysis of ion implantation phenomenon by two-body scattering model

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In the previous our articles about ion implantation, we have introduced the contents specialized in compound semiconductors. This time, we will introduce the matters related to the analysis of basic channeling implantation into silicon and review the commentary articles so far. We also inform on the challenges of commonly used analysis codes for ion implantation phenomena.

In this article, we explain the following contents.

1. Channeling implantation profile into silicon

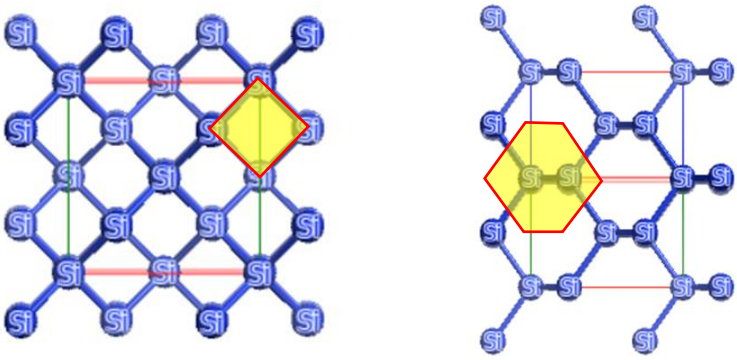
2. Stopping power

3. Future issues

1. Channeling implantation profile into silicon

Silicon crystal has a diamond structure. Figure 1 shows the arrangement of silicon atoms as seen from the (001) and (110) planes (1). The horizontal axis represents the a-axis. In other words, the figure on the left side corresponds to channeling injection along the axis of [001]. The figure on the right side shows the arrangement of silicon atoms as seen from the (110) plane.

Fig. 1:Crystal structure of silicon [left:(100) right:(110)]



As a review of our previous commentary articles, we will give an overview of the analysis when boron is implanted into silicon. The model of electronic stopping power is an important factor in predicting the depth distribution of channeling implanted ions. Models of the non-local stopping power proportional to the flight distance of incident ions at the target and the local stopping power depending on the collision coefficient have been proposed. The non-local electronic stopping power is expressed by the following equation.

$$\Delta E^{nl} = x^{nl}\, N\, S_e\, L$$

The N is the atomic density of the target, $x^{nl}$ is the percentage of non-local electronic stopping power, and Se is the electronic stopping power of random implantation (2).

On the other hand, the Oen-Robinson model, which depends on the impact parameter as follows, is adopted for the local electronic stopping power (3).

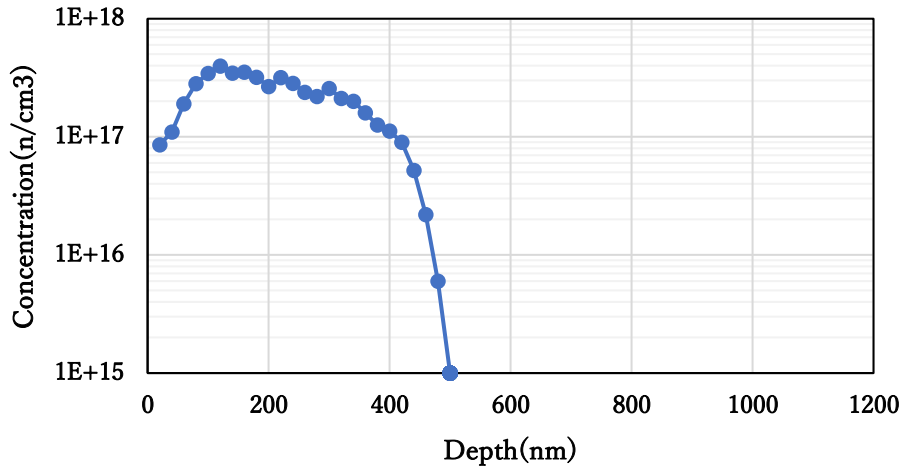
$$\Delta E^{loc} = (1 - x^{nl}) \frac{S_e}{2\pi a^2} exp\left(-\frac{p}{a}\right)$$

Here, *p* represents the impact parameter and *a* represents the shielding length.

It is known that random implantation does not depend on the ratio of non-local electronic stopping power and the shielding length. However, according to previous reports, it is necessary to adjust the ratio of non-local electron stopping power and the value of shielding length in order to match the analysis result of channeling implantation into the (100) and (110) planes with the result of SIMS (4).

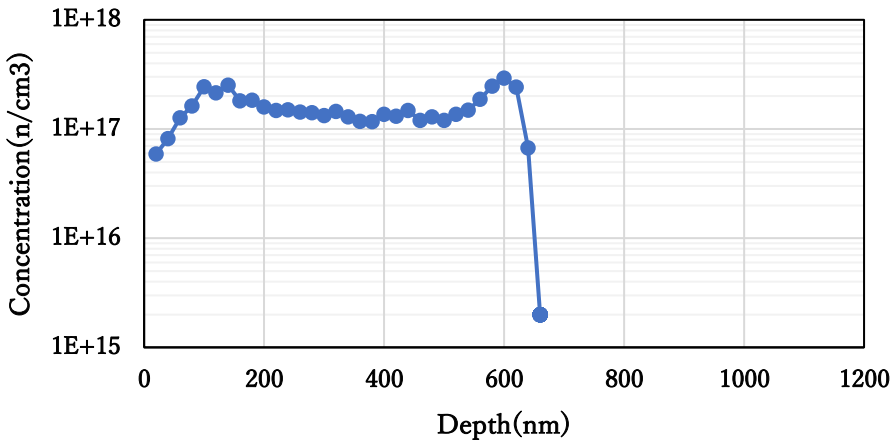
Furthermore, it is necessary to set the value of the Debye temperature, which is related to the lattice vibration of silicon, to the optimum value. It has been reported that the profile reproducibility of channeling implantation was improved by selecting the optimum values (5). Figure 2 shows the analysis results of the channeling implantation of 20 keV boron ion into Si (100). This result is consistent with the SIMS result.

Fig. 2 : B20keV→Si(100) 1E13/cm2



On the other hand, in the channeling implantation into the (110) plane, as shown in Fig. 3, it can be seen the boron has penetrated deeper than the (100) plane. This result is due to the fact that the (110) plane has a larger open space cross-section in the arrangement of silicon atoms than the (100) plane.

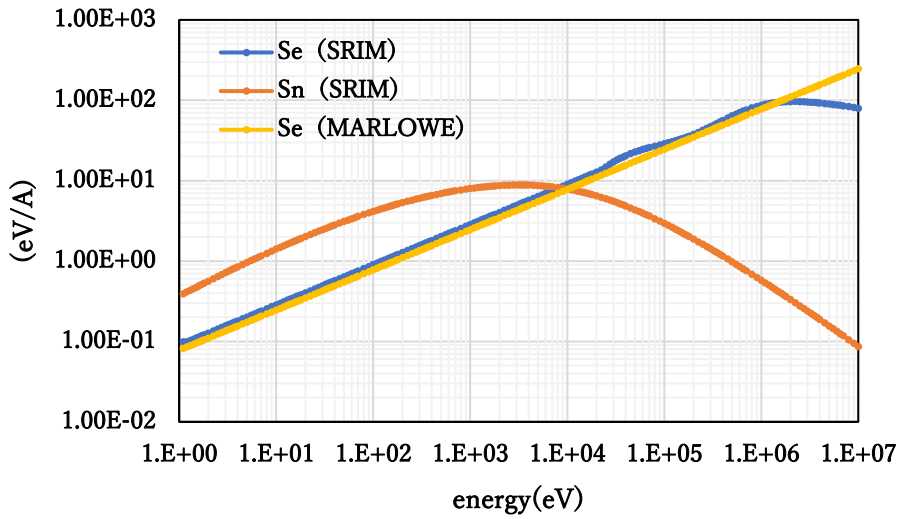
Fig. 3：B20keV→Si(110) 1E13/cm2



## 2. Stopping power

Figure 4 shows a graph of electronic stopping power and nuclear stopping power when boron is implanted into silicon as determined by SRIM. It can be seen that the electronic stopping power becomes dominant when the incident energy is 10 keV or higher. The electronic stopping power value obtained by SRIM, and the electronic stopping power value obtained by MARLOWE can be matched by multiplying by a small correction factor up to about 2 MeV.

Fig. 4：Stopping power (B-Si)

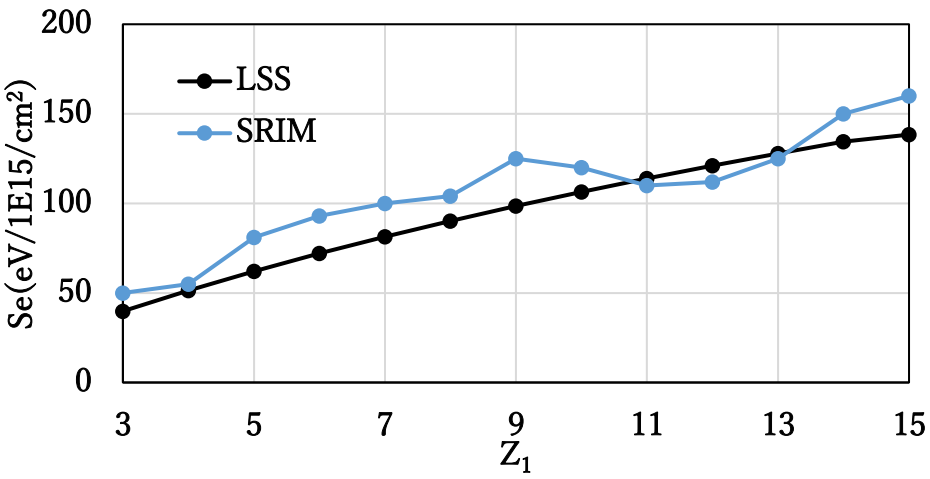



In other words, up to this energy, the classical LSS theory that the electronic stopping power is proportional to the square root (velocity) of the incident energy can be explained. However, a model (Bethe-Bloch) is required in which the stopping power decreases in inverse proportion to the incident energy when the incident energy exceeds 2 MeV. In general, the stopping power is proportional to $V^{-2}$ in the region of $V >> Z^{2/3} \times v_0$. On the other hand, in the region of $V << Z^{2/3} \times v_0$, the stopping power is proportional to V. Here the $v_0$ is Bohr velocity.

## 3. Future issues

As explained earlier section, the two-body scattering can basically be described by classical LSS theory, but in reality, there are limits. In the field of ion collision, it is known that the electron stopping power changes depending on the atomic number of the incident ion. This phenomenon is called as $Z_1$ oscillation (6). As shown in Fig. 5, the electron stopping power obtained by LSS theory and the electron stopping power obtained by SRIM are compared for atomic number $Z_1$. The target is assumed to be a silicon atom.

Fig. 5：Electronic stopping power




From Fig. 5, it is clear the electronic stopping power oscillates as the atomic number increases. This phenomenon cannot be reproduced by LSS theory. Therefore, a new collision model has been proposed to explain the atomic number dependence of electronic stopping power (7). For example, the following equation has been proposed as a model of electronic stopping power.

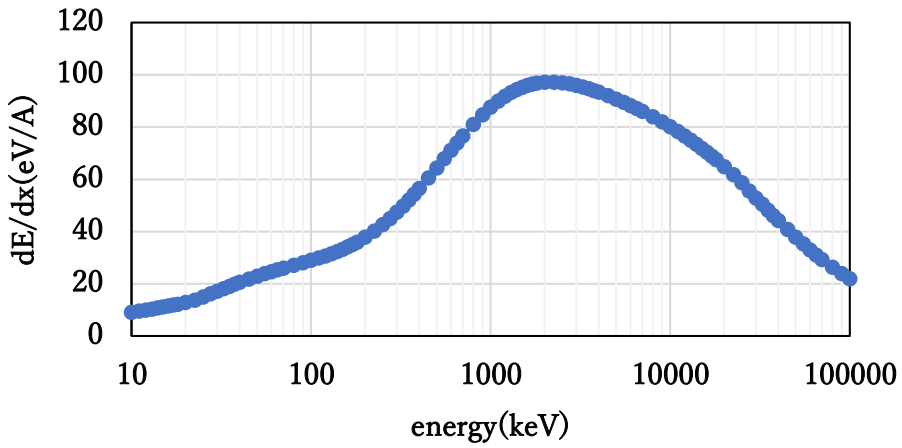
$$S_{non-local} = \int [Z_1^*(v, r_s^0)]^2 \, S_p(v, r_s) dx$$

$Z_1^*$: effective charge of incident ion
$S_p$: electronic stopping power of proton
$r_s^0$ : radius of electron
v : velocity of primary ion

It has been reported that this model requires a huge amount of calculation time because it is necessary to calculate the electronic stopping power for the orbit of all ions.

Therefore, some group imports SRIM's electronic stopping power database and perform analysis in a more realistic calculation time (8). They are obtaining the stopping power at any energy by curve-fitting the stopping power data obtained from SRIM by the combination of incident ion and target material. Figure 6 shows the energy dependence of the electronic stopping power when B ions are incident on Si. It can be seen that the stopping power value decreases with energy at the energy of 3000 keV or higher. This trend is explained in Section 2.

Fig. 6 Electronic stopping power(B→Si)




In order to perform such a general-purpose ion implantation simulation, the key point is how accurately the electronic stopping power can be handled. In order to solve this problem in the future, it is necessary to proceed with the study with a view to updating the program.

Supplementary explanation of LSS theory

It is a theory that assumes that the velocity scaling law holds for the electron stopping power and the energy scaling rule holds for the nuclear stopping power in the collision system between the incident ion and the target atom. It is named as LSS theory using the acronym of the researcher who proposed this theory (Lindhard-Sharff-Shiott). It is assumed that these two stopping powers can be separated and atomic collisions can be analyzed.

**References**

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