Comparison of modified Firsov & Hobler model for channeling implantation analysis

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Introduction

For the past few years, we have been analyzing the phenomena related to channeling ion implantation using the MARLOWE code. We have mainly focused on comparing channeling phenomena in compound semiconductors such as 4H-SiC and GaN with SIMS profiles [1, 2]. In this explanatory article, we re-examine the analytical model that forms the basis of channeling simulations and present the results of our attempt to evaluate the electronic stopping power in channeling implantation.

As a model for dealing with channeling phenomena, the Firsov model was proposed in the 1950s, which models electron transport phenomena by assuming the overlap of the target electron cloud and the incident ion's electron cloud [3]. El-Hoshy and Gibbons extended this model to propose a model that can reproduce the atomic number dependence of electronic energy loss in the incident ion, i.e., Z1 oscillations [4]. Meanwhile, Oen-Robinson also proposed the analytical model that deals with the interaction between the incident ion and the electrons of the target atom [5]. Robinson developed the MARLOWE code by adopting the LSS model and the Oen-Robinson model [6]. Hobler improved the analytical model of the MARLOWE code to develop the IMISIL code [7]. Furthermore, Tian developed a TCAD simulation code that adopts Hobler's analytical model [8]. These simulation codes cannot directly handle the Z1 oscillation phenomenon, but they contribute to the reproduction of SIMS profiles by optimizing collision-related parameters [9].

This article explains the method for extending Hobler's analytical model using the channeling profiles measured by SIMS to determine electronic stopping power. We also compare this result with the electronic stopping power obtained by using the El-Hoshy-Gibbons model. In channeling implantation into SiC, light elements tend to have higher concentrations in deeper profiles. Similarly, in channeling implantation into GaN, light elements tend to have higher concentrations in deeper profiles. This trend is also considered from the perspective of electronic stopping power. While several mathematical formulas are included, explanations are provided to ensure understanding of their derivations. Furthermore, numerous graphs are used to facilitate comprehension. Please read to the end.

Energy loss by Hobler model

Hobler assumed non-local energy loss, which is independent of the incident ion's position, and local energy loss, which is dependent on the incident ion's position. He proposed a model that reproduces the channeling profile by adjusting the ratio of each component (x^{nl} & x^{loc}). The analytical formula for the model is shown below. Electronic energy loss can be expressed as the sum of non-local and local energy loss by the following formula.

$$\Delta E_e = \Delta E_e^{nl} + \Delta E_e^{loc}$$

The non-local energy loss is expressed by the following formula.

$$\Delta E_{nl} = N\, S_e\, \Delta R \left[x^{nl} + x^{loc} \left(1 + \frac{p_{max}}{a}\right) exp\left\{-\frac{p_{max}}{a}\right\}\right]$$

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

$$x^{nl} + x^{loc} = 1$$

$$a = \frac{a_{12}}{\gamma}$$

Here, Se represents the electronic stopping power based on the LSS theory. p_{max} is the maximum value of the collision coefficient, a_{12} is the shielding length, and γ is the adjustment parameter for the shielding length.

Meanwhile, the local energy loss at impact parameter p is expressed by the following equation based on the Oen-Robinson model.

$$\Delta E_{loc} = x^{loc}\, \frac{S_e}{2\pi a^2} exp\left\{-\frac{p}{a}\right\}$$

Energy loss by El-Hoshy and Gibbons model

El-Hoshy and Gibbons improved the Firsov model, which deals with the interaction between electrons of an incident ion and electrons of a target atom, to propose a model that can handle Z1 oscillations. The electronic energy loss in this model is expressed by the following equation [4].

$$\Delta E = \frac{4.3 \times 10^{-8}(Z_1' + Z_2' - 1)^{5/3} \times v}{\left[1 + 0.15(Z_1' + Z_2' - 1)^{1/3}\left(\frac{R_0}{a_0}\right)\frac{1}{y}\right]^5}$$

Here, v is the velocity of the incident ion, R_0 is half the channel width, a_0 is the Bohr radius, and y can be given as a parameter. This y is set to 5 if the atomic radius of the incident ion is greater than R_0, and to 10 if the atomic radius of the incident ion is less than R_0.

Z_1 and Z_2 represent the atomic number of the incident ion and the target atom, respectively. The primed atomic number is a value proposed that takes into account the occupancy of the outermost electron shell. For example, in the case of oxygen, the number of electrons in the outermost shell, i.e. L shell, is 6. A maximum of 8 electrons is allowed in the L shell. Since the number of outermost electrons is greater than half the maximum number of electrons in the L shell, i.e. 4, the following value is set as the effective atomic number [4].

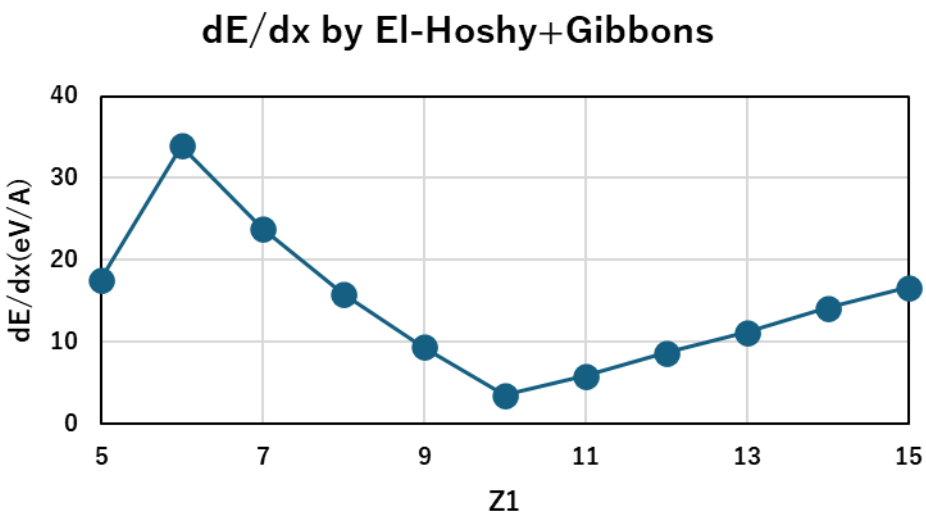
Z‘=6-2(6-4)=2

The electronic stopping power per length can be calculated using the following formula.

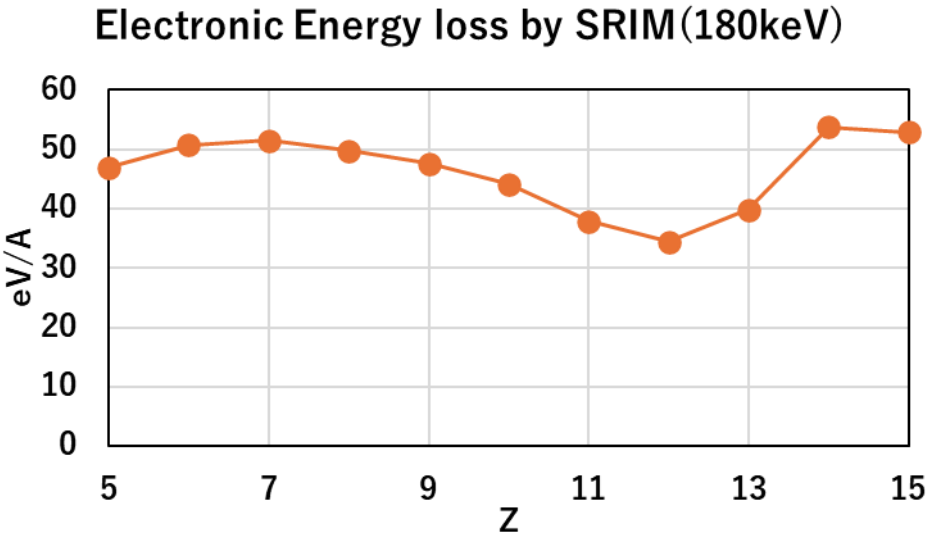
$$\frac{dE}{dx} = \frac{1}{W} \times \frac{4.3 \times 10^{-8}(Z_1' + Z_2' - 1)^{5/3} \times v}{\left[1 + 0.15(Z_1' + Z_2' - 1)^{1/3}\left(\frac{R_0}{a_0}\right)\frac{1}{y}\right]^5}$$

Here, W represents the distance between atoms in the direction of the incident ion’s movement.

The dependence of the electronic stopping power on the incident ion's atomic number in the case of ion implantation into GaN, as determined by this expression, is shown below.

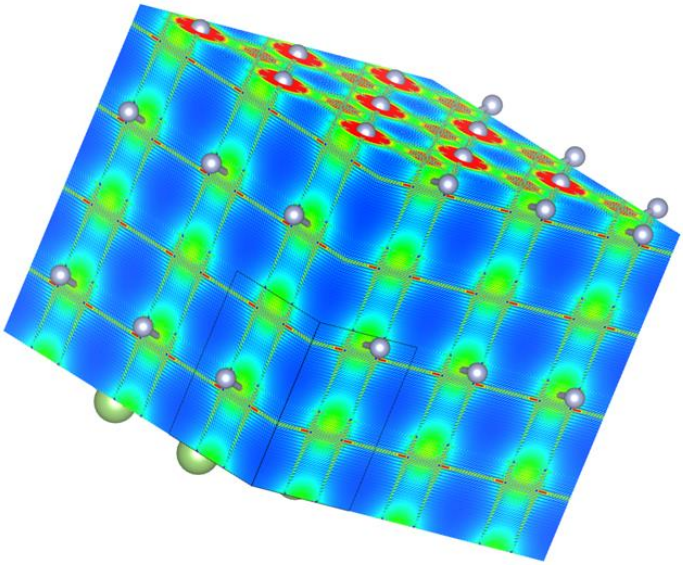


This successfully represents the change in electronic stopping power with respect to the atomic number Z_1 of the incident ion. The graph below shows the Z_1 dependence of the electronic stopping power obtained by the SRIM code. Compared to the previous dependence of stopping power, the amplitude of the Z_1 oscillation is larger for channeling ion implantation. This suggests that the influence of the outermost electrons of the incident ions is significantly evident.

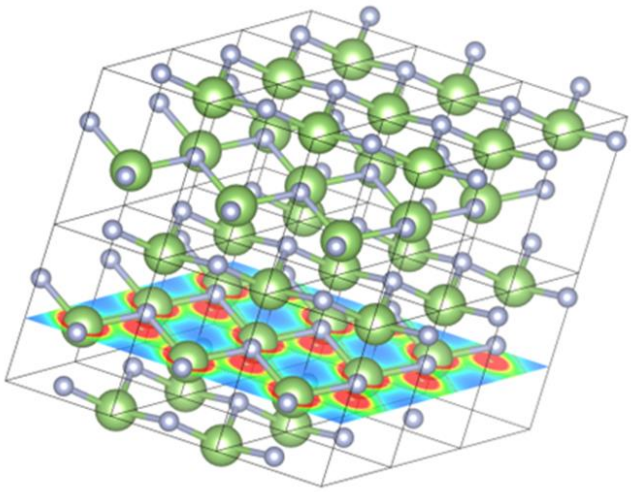


Estimation of electron density distribution by VESTA

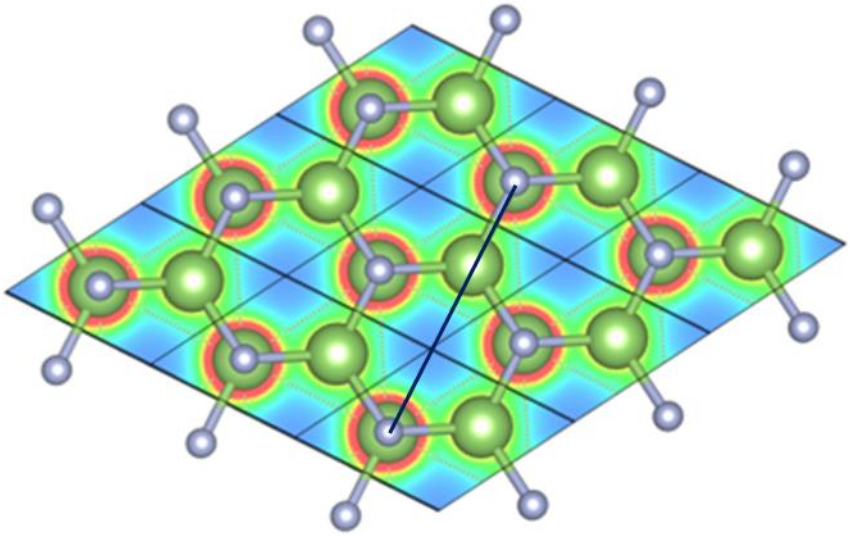
A code capable of 3D visualization of crystal structures has been released [10]. This code can display the electron density distribution in 3D using data from first-principles calculations and X-ray diffraction data. Alternatively, the electron density distribution can be analytically determined by Fourier transformation using the structure factor of the target atom. In the 3D visualization of the GaN crystal structure below, the large green spheres represent Ga atoms, and the small gray spheres represent N atoms.



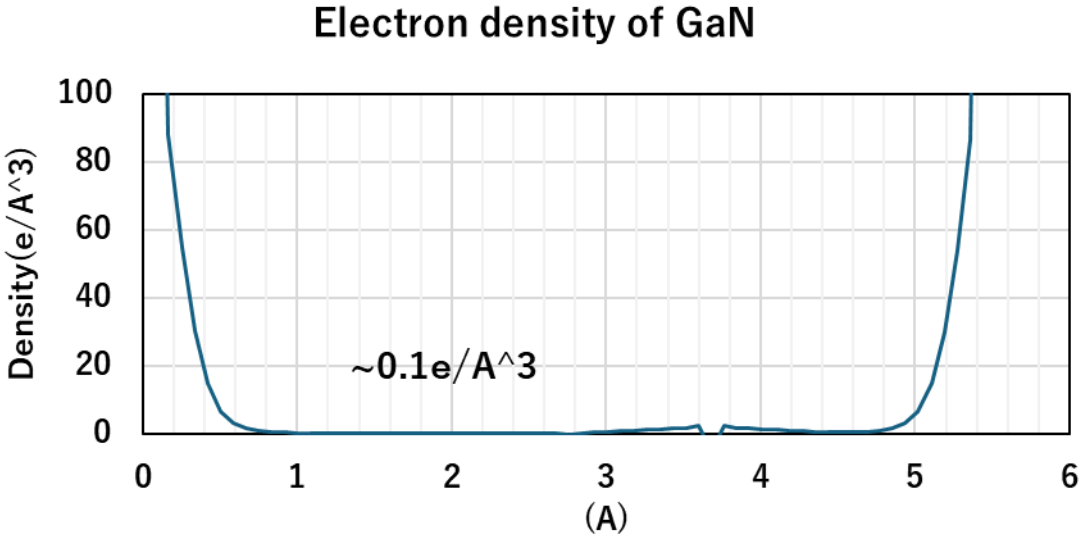
The electron density distribution across a specific crystal plane crossing a Ga atom is shown below. Red color indicates high-density regions, and blue color indicates low-density regions.



We determined the linear distribution of electron density along the dark blue line drawn on the electron density distribution shown in the figure below.



The graph below shows the electron density distribution. The horizontal axis represents the distance between Ga atoms, and the vertical axis represents the electron density distribution. From this graph, it can be seen that the electron density increases sharply near the Ga atoms. The electron density near the crystal center axis is approximately 0.1e/A^3. From this graph, it can be inferred that when the incident ion and the target atom approach each other to about 1 Å, the influence of the inner-shell target electrons will be significant.



Estimation of electronic stopping power

The electronic stopping power is expressed by the following formula.

$$\frac{dE}{dx} = \frac{dE_{nl}}{dx} + \frac{dE_{loc}}{dx}$$

Each electronic stopping power is as follows.

$$\frac{dE_{nl}}{dx} = N\,S_e \times \left[x^{nl} + x^{loc}\left(1 + \frac{p_{max}}{a}\right)\,exp\left\{-\frac{p_{max}}{a}\right\}\right]$$

$$\frac{dE_{loc}}{dx} = x^{loc}\,\frac{S_e}{W\,2\pi a^2} \times \left[\,exp\left\{-\frac{p_{max}}{a}\right\}\right]$$

Generally, the range is the average distance a particle with energy E_0 travels before it loses energy and effectively stops moving. While there are several definitions of range, here we have adopted the CSDA range. CSDA stands for Continuous Slowing Down Approximation, and it is the range calculated assuming the particle travels in a straight line and continuously loses energy gradually. In the case of channeling injection, since the particle travels almost in a straight line along the channeling axis, this definition is considered appropriate.

The total electronic stopping power is expressed by the following equation

$$\frac{dE}{dx} = S_e \times \left[N\left\{x^{nl} + (1 - x^{nl})\left(1 + \frac{p_{max}}{a}\right)exp\left(-\frac{p_{max}}{a}\right)\right\} + \frac{(1 - x^{nl})}{W}\;\frac{1}{2\pi a^2}\,exp\left(-\frac{p_{max}}{a}\right)\right]$$

In this equation, Se is the square root of energy, so we can rearrange the equation to express it as an integral of energy, corresponding to the integral of distance. The position where the energy of the incident ion becomes zero is the maximum distance the incident ion can reach.

$$R_{max} = \int_0^{R_{max}} dx$$

$$= \int_{E_0}^{0} \frac{dE}{k\sqrt{E}\left[N\left\{x^{nl} + (1 - x^{nl})\left(1 + \frac{p_{max}}{a}\right)exp\left(-\frac{p_{max}}{a}\right)\right\} + \frac{(1 - x^{nl})}{W}\,\frac{1}{2\pi a^2}exp\left(-\frac{p_{max}}{a}\right)\right]}$$

The performing this integral gives the following simple result.

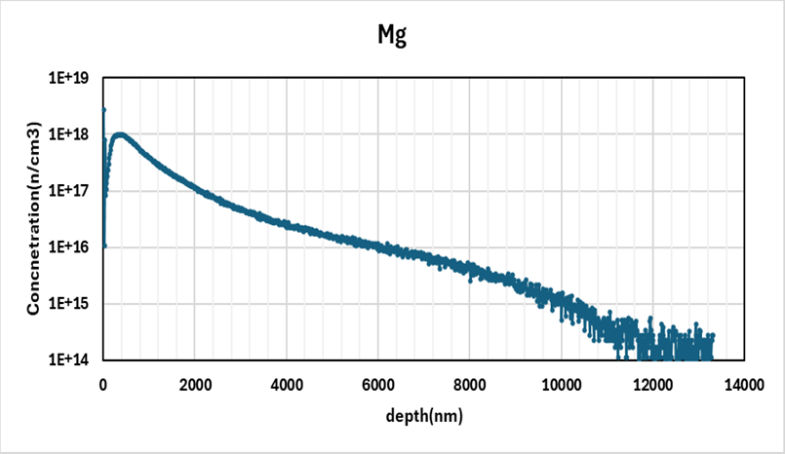
$$R_{max} = \frac{2\sqrt{E_0}}{K}$$

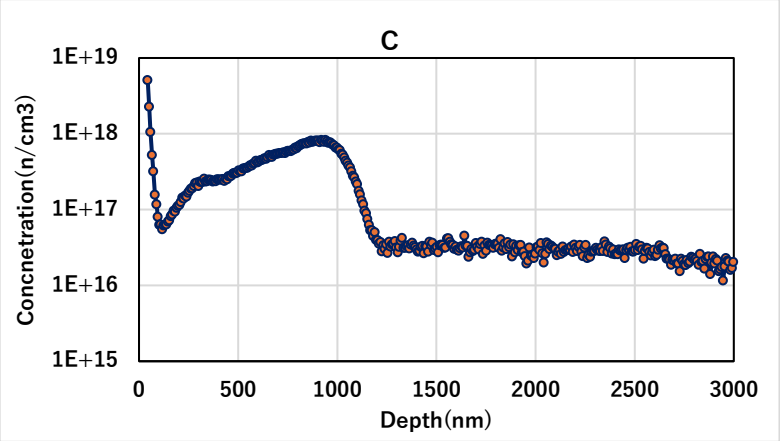
$$K = k\left[N\left\{x^{nl} + (1-x^{nl})\left(1+\frac{p_{max}}{a}\right)exp\left(-\frac{p_{max}}{a}\right)\right\} + \frac{(1-x^{nl})}{W}\ \frac{1}{2\pi a^2}exp\left(-\frac{p_{max}}{a}\right)\right]$$

The p_{max} in this formula can be considered as the distance at which the interaction between the incident ion and the electron cloud of the target atom has an effect. In this article, the value was determined by referring to the average atomic radius of GaN.

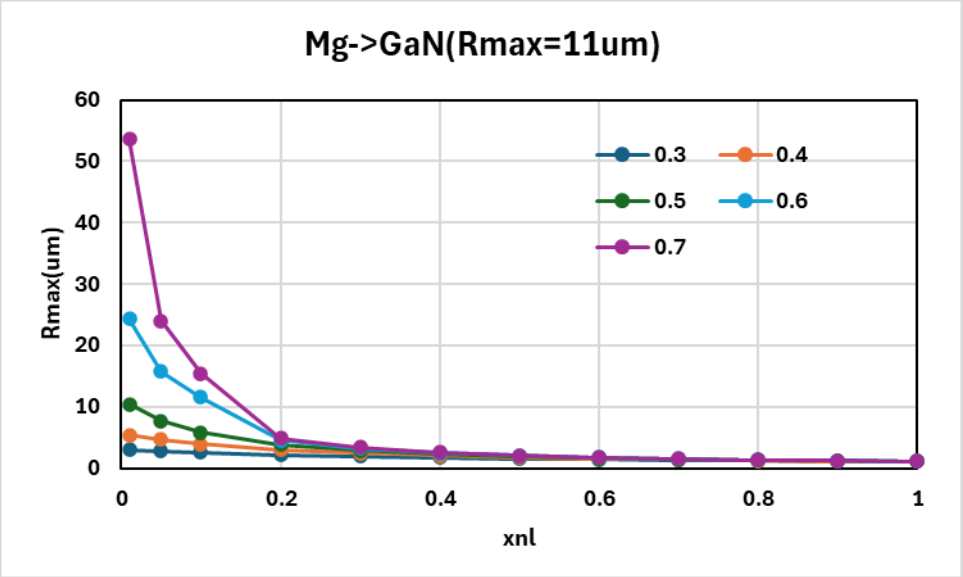
In this article, R_{max} is defined as the position at which the profile obtained by SIMS reaches the background. Some reports use the depth at which the concentration decreases to 10% of the maximum concentration. However, since the differences in profiles due to the type of incident ion may not be represented at R10%, we used the position at which the profile reaches the background level for our analysis.

The SIMS profiles when 180keV Mg and C are implanted into the GaN (0001) plane are shown.

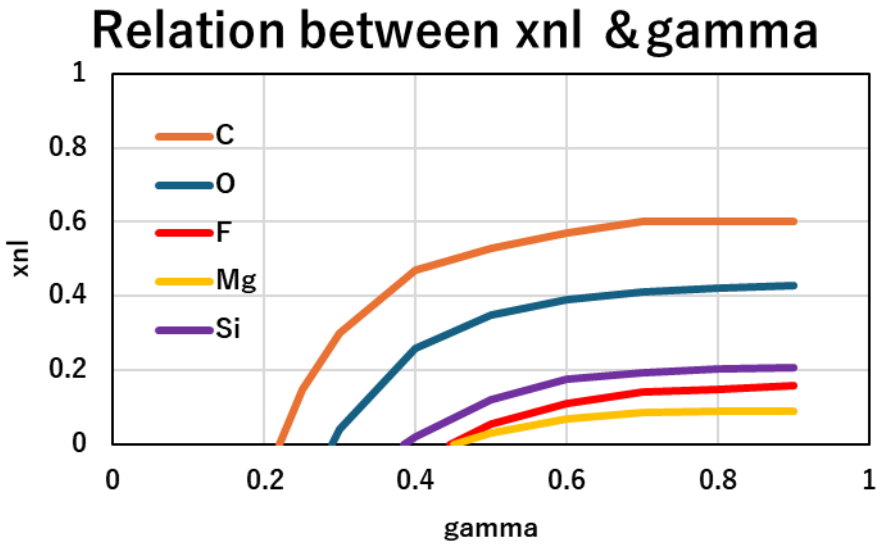




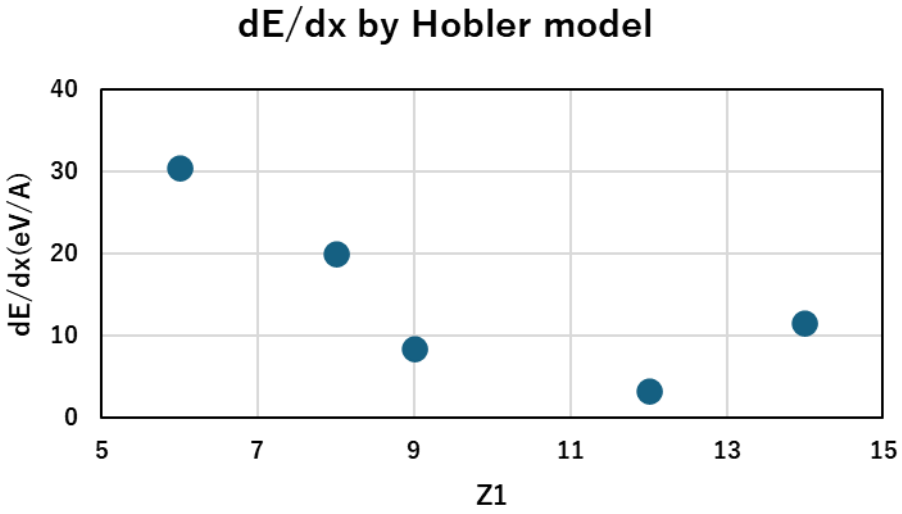
We determined R_{max} and sought combinations of γ and x^{nl} that satisfy the value of R_{max}. The ratio of non-local energy loss x^{nl} contributes to making the channeling profile shallower, while γ contributes to broadening the tail of the channeling profile. This trend can be seen in the graph below. As can be seen from the formula described earlier, the value of the electronic stopping power is the same regardless of the combination of γ and x^{nl} if R_{max} is satisfied.



However, when x^{nl} is zero, the value of γ that satisfies R_{max} has the minimum, and as γ increases, x^{nl} also increases, as can be seen from the following graph. The results of similar analysis for other ion species are shown in the following graph. It was also confirmed that the combinations of γ and x^{nl} obtained for reproducing the SIMS profile using the fitting by MARLOWE lie on these curves.



We determined the value of the electronic stopping power by defining R_{max}. The results are shown in the following figure.



As shown in the table below, the values of the electronic stopping power obtained from the El-Hoshy-Gibbons model are in close agreement.

	Se by Hobler(eV/A)	Se by HG(eV/A)
C	32	34
O	20	16
F	9	9.4
Mg	3	8.7
Si	12	14

The channeling profile of Mg extends to about 10 microns, but for the light element C, it only extends to about 1 micron at the same energy. This is because the electron stopping power of C is about ten times greater than that of Mg, making C more prone to losing energy. As a result, the channeling profile is shallower compared to Mg. Furthermore, to clarify the trend of changes in the

channeling profile due to the incident ion, we considered the ratio of the electron stopping power obtained from SRIM to the electron stopping power in channeling injection obtained in this study. From the simplified R_{max} formula, the ratio of the maximum range of random and channeling is the reciprocal of the ratio of electron stopping powers.

$$\frac{R_{max}^{ch}}{R_{max}^{ran}} = \frac{K_{ran}}{K_{ch}}$$

In other words, if the electronic stopping power of channeling is very small compared to random channeling, the channeling tail will extend deeper than the random peak in the channeling profile. On the other hand, if the ratio of electronic stopping powers is the same order, the extension of the channeling tail will be smaller compared to the random peak.

	Se by Hobler(eV/A)	Se by SRIM(eV/A)	Se(SRIM)/Se(Hobler)
C	32	50	1.6
O	20	50	2.5
F	9	48	5.2
Mg	3	35	12
Si	12	52	4.3

From these calculation results, we can see that in C implantation, the electronic stopping power of channeling is close to that of random, so the channeling peak is located slightly deeper than the random peak. On the other hand, in Mg implantation, the electronic stopping power of channeling is much smaller than that of random, so channeling ions tend to penetrate deeper into the region.

Summary

We revised the analytical model underlying the simulations using the MARLOWE code. It was estimated that the reason the channeling profile differs depending on the incident ion is due to the oscillation of the electronic stopping power depending on the atomic number of the incident ion. Actual calculations using the El-Hoshy-Gibbons model, an improved version of the Firsov model, confirmed a correspondence between the values of electronic stopping power obtained from the Hobler model using R_{max}. The tendency for the channeling profile concentration distribution to reverse in light element ion implantation was estimated by comparing the electronic stopping powers of channeling and random implantation. This article introduced how the atomic number dependence of the SIMS profile due to incident ions could be expressed from the analytical formula for electron energy loss underlying the channeling simulation. Thus, while the MARLOWE code can reproduce SIMS profiles in ion implantation into crystals, the understanding of the underlying analytical model is necessary. The parameter for non-local energy loss can be said to be the distinction between whether the electron cloud of the target atom affects the incident ions or not. This distinction is determined by the impact parameter p. We assume that incident ions at positions smaller than the collision coefficient p_{max} experience local energy loss, while ions incident at positions greater than p_{max} experience non-local energy loss. Ultimately, parameters such as x^{nl} that can reproduce the SIMS profile are adjusting the stopping power value.

References

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