Channeling simulation using a damage accumulation model

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Introduction

A few years ago, we introduced the MARLOWE code that has been developed at Oak-ledge national laboratory at United States [1]. So far, we have analyzed channeling profiles in the low dose region with few defects in 4H-SiC, GaN, and Si [2]. When the implantation dose increases, interstitial atoms dislodged by the implanted ions accumulate within the crystal axis. This causes channeling to be hindered. To reproduce this phenomenon through simulation, we must preserve the defect information formed by ion implantation and deal with the phenomenon in which the incident ions are scattered by the defects.

The injection of a single ion forms hundreds of pairs of interstitial atoms and vacancies. These are called Frenkel pairs. In an actual analysis, it is necessary to save all information such as the coordinates of all Frenkel pairs. This method had the problem that the analysis time was too long, and the amount of defect data output was huge. Furthermore, the MARLOWE code itself was old, so there was a limit to the amount of information it could handle. Therefore, we re-examined the damage accumulation model of the MARLOWE code and revised the collision phenomenon so that the analysis could be performed within the limits of the MARLOWE code. As a result, it became possible to analyze the change in the channeling profile for a specified dose range.

On the other hand, it is known that an amorphous oxide film of a few angstroms is formed on Si and 4H-SiC [3]. However, NIMS and North Carolina University have reported that an extremely thin oxide film (0.6-1.0 nm) in a crystalline state is formed on the surface of GaN [4, 5]. They prepared samples of about 5 nm thickness by ion milling with minimal damage to the GaN surface and reported atomic-level arrangement information by high-resolution STEM. The crystal structure is estimated to be stable β-type gallium oxide or metastable κ-type gallium oxide.

Based on the above background, we will explain the outline of the damage accumulation model by taking the channeling implantation of boron into silicon as an example. Using a defect generation model, we will explain the behavior of how the amount of defects generated increases with incident energy. The simulation was performed assuming that the GaN surface is β-type gallium oxide in a crystalline

state. We will show the results of a simulation of how the channeling profile changes depending on the dose, and the depth distribution of the ratio of Frenkel pairs generated by ion implantation to the GaN atom number density.

Finally, regarding the dose dependence of the channeling profile, we set a virtual amorphous layer on the substrate surface and adjusted the amorphous film thickness so that the channeling profile measured by SIMS can be reproduced[6]. We will show the results of our investigation into how this virtual amorphous film can affect the energy and scattering angle of primary ion. Finally, we introduce the model that the defect density is depend on the square root of dose.

- Overview of damage accumulation model
- Frenkel pair generation model
- Consistency between β-type gallium oxide and gallium nitride
- Dose amount and channeling profile
- Effect of a virtual amorphous layer to the characteristics of primary ion

Damage accumulation model

The following are the basic parameters required for analysis using the damage accumulation model. First, determine the dose you want to analyze, and then calculate the number of incident ions (NI) per implant area (S).

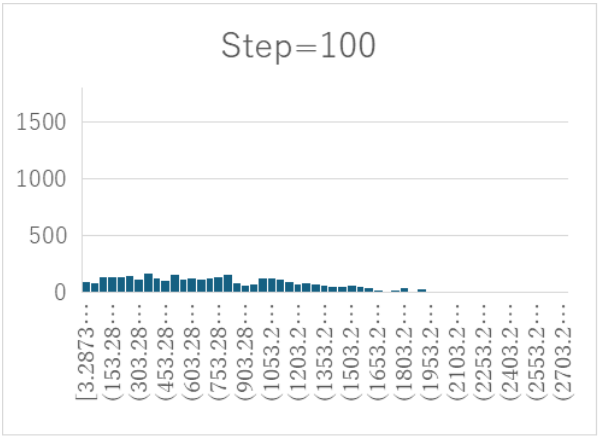
$$Dose = \frac{NI}{S}$$

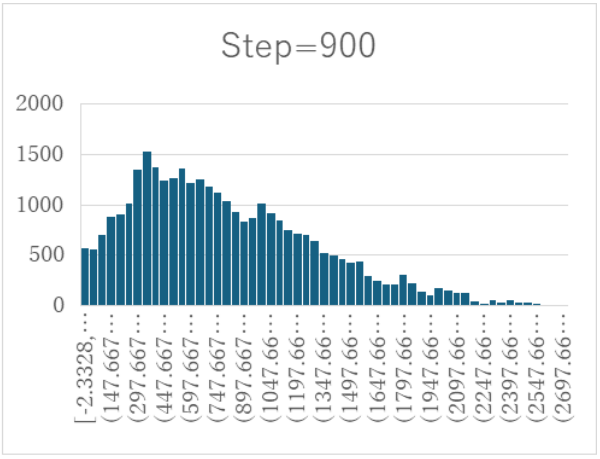
The calculation process will be explained using the case where NI = 10 as an example. One ion is implanted into a target without defects, and the coordinates of all pairs of interstitial atoms and vacancies created, that is, Frenkel pairs, are saved. Next, a second ion is implanted into the target with defects, and the Frenkel pair information is saved. This process is repeated up to 10 ions. To improve statistical accuracy, the process of implanting 10 ions is repeated 1,000 times, resulting in a profile being obtained using 10,000 incident ions.

We evaluated the channeling implantation profile to see if MARLOWE could analyze damage. As an example, we will explain the case of channeling implantation of 15 keV boron into silicon. The target setting assumes an amorphous film of 10 Å on the surface. It is estimated that the broad peak seen around 80 nm from the surface

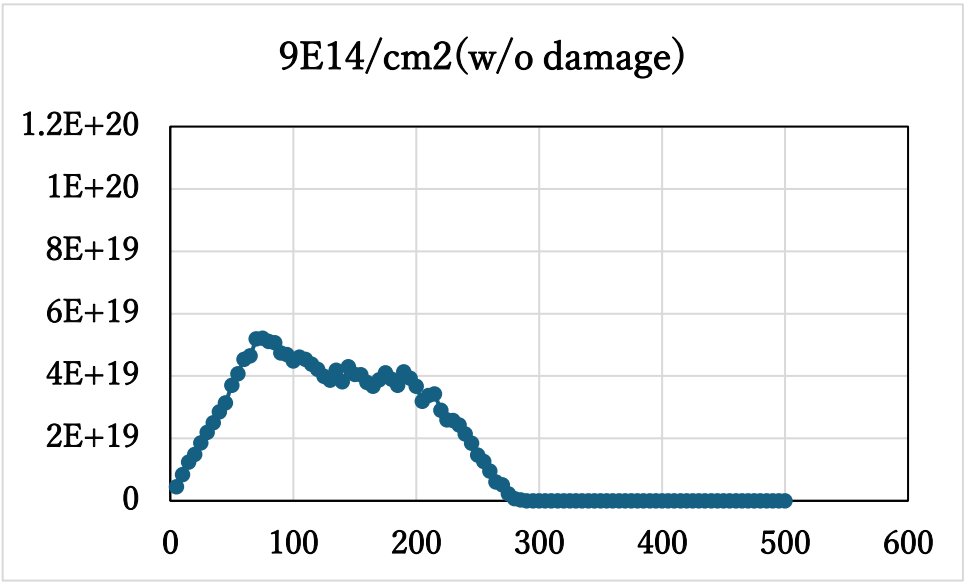
when damage is not taken into account (w/o damage) is due to the effect of surface oxidation. Researchers at the Royal Institute of Technology in Sweden, who are studying channeling implantation into 4H-SiC, have also been able to reproduce the shape of the channeling profile by assuming an 8Å oxide film on the surface [1].

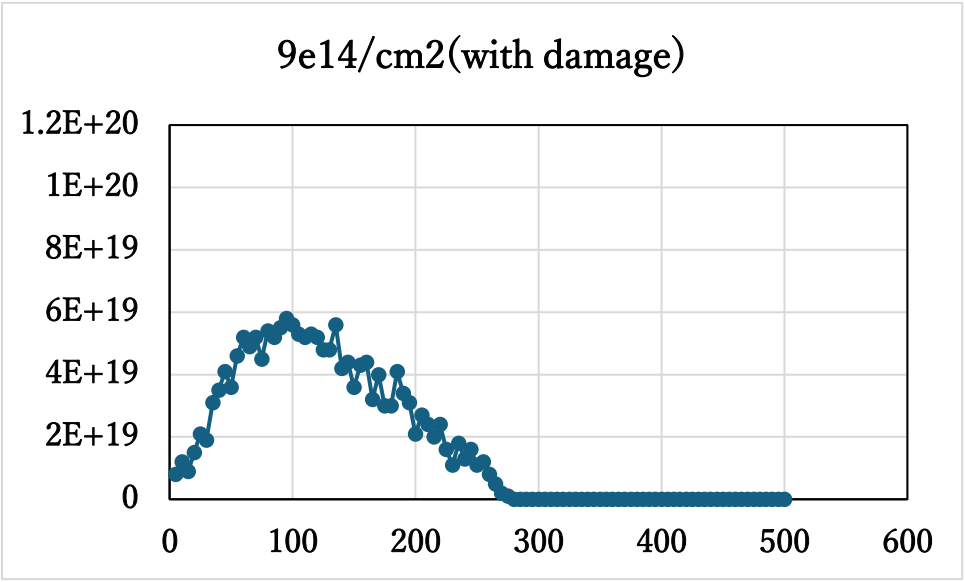
As the dose increases, silicon atoms in the crystal lattice are dislodged due to scattering by the incident ions, becoming interstitial atoms. The figure below shows the distribution of interstitial silicon in the depth direction when 100 ions are incident and when 900 ions are incident. It is clear that the number of interstitial atoms increases as the number of incident ions increases.

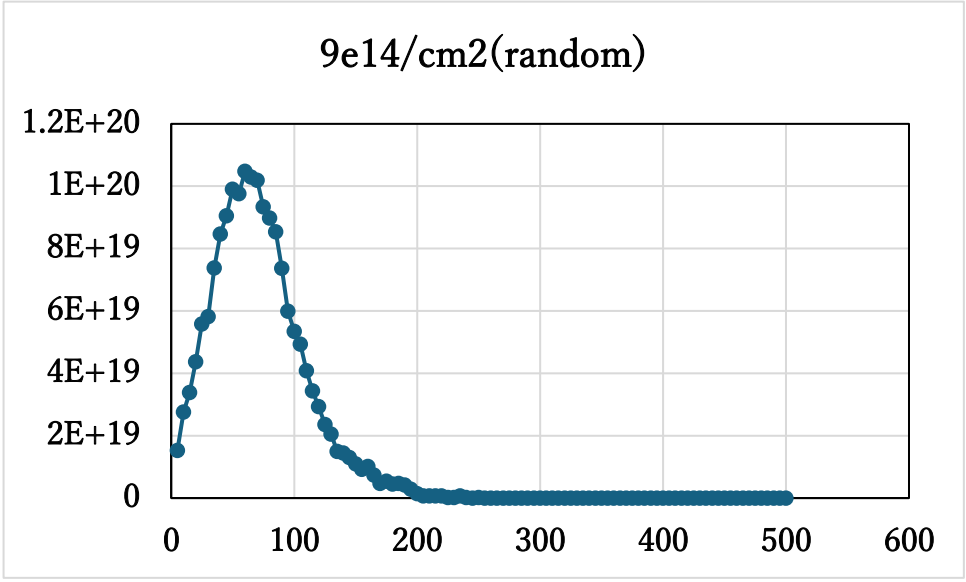




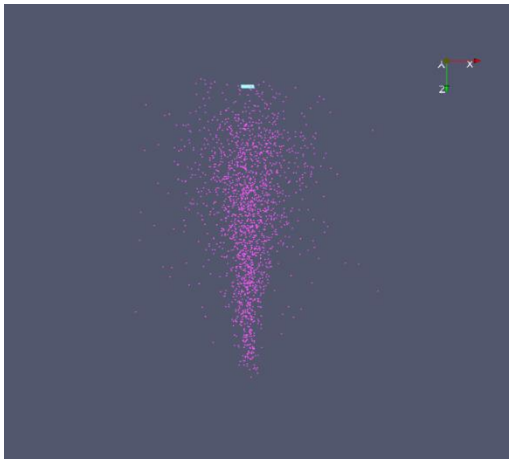
The channeling of incident ions is hindered by the interstitial atoms that now exist on the crystal axis. This phenomenon is called dechanneling. This phenomenon causes incident ions to stop closer to the surface than in the case of channeling. As a result, as the dose increases, the peak at the surface becomes higher and the profile becomes broader in the depth direction. This phenomenon is explained in the following figure. The profile when damage is taken into account (with damage) has a broader shape than the peak when damage is not taken into account. In other words, it can be seen that MARLOWE reproduces the dechanneling phenomenon caused by the accumulation of interstitial atoms. As the dose increases, the position of the peak approaches the value in the case of random implantation.

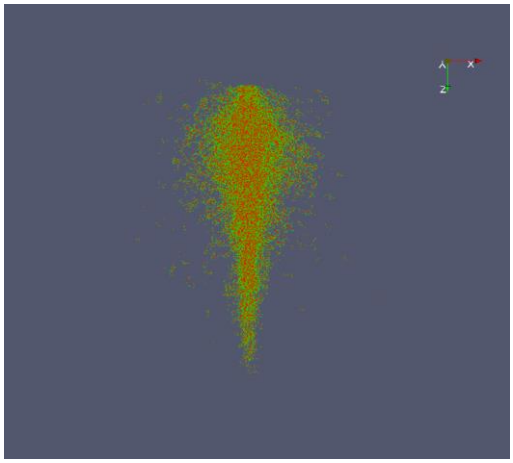




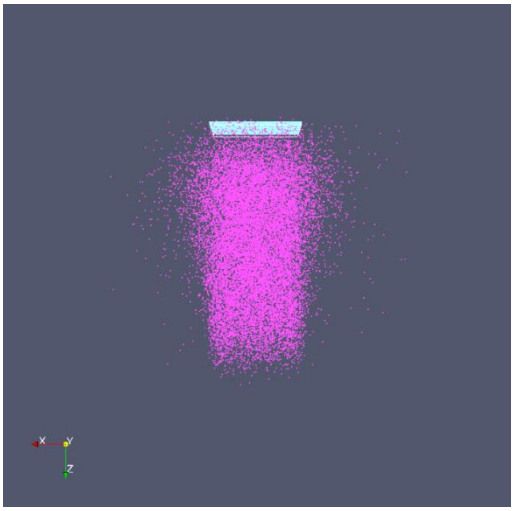


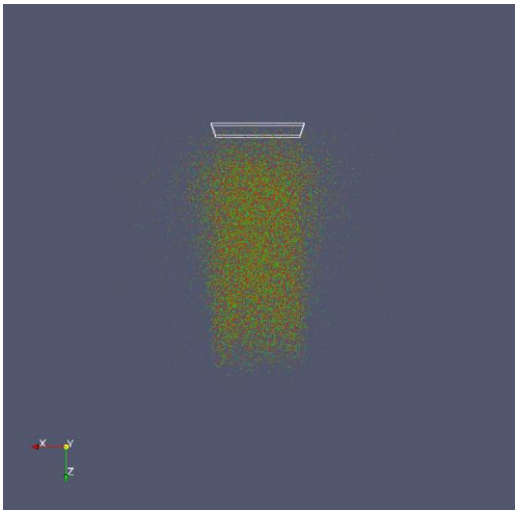
The following graphs show a 3D display of the depth distribution of ion-implanted atoms. The figure on the left shows the depth distribution of boron, the incident ion. The light blue area shown in the figure shows the distribution of the incident ions. The irradiation area is set to a 10 nm square. The figure on the right shows the depth distribution of Frenkel pairs generated by ion irradiation. These distribution figures show that both the incident ions and Frenkel pairs are distributed horizontally over several tens of nm or more. The difficulty with damage analysis is that it often underestimates the effects from areas far away from the area irradiated by the incident ions.





The profile when the irradiation area is set to 100 nm square is shown below. Robinson, the developer of MARLOWE, recommends extracting information from the central area from the distribution shown below and analyzing the damage. However, this is not a realistic method because it requires long calculation time and large output capacity. A research group in Spain has modified the analysis code to limit the irradiation area, fold back ions that leave the irradiation area, and track the ion trajectories to take into account collision phenomena [7].





Frenkel pair production model

The NRT (Norgett-Robinson-Torrens) model is a theoretical model that predicts the amount of atomic displacements that occur in materials due to radiation exposure [8]. Specifically, it is a method for numerically analyzing damage caused by atomic collisions (cascade damage). The mathematical expression of this model is shown below.

$$Frenkel\ pairs(E_p) = \frac{0.8}{2E_d} E_D$$

$$E_D = \frac{E_p}{1 + k\ g(\varepsilon)}$$

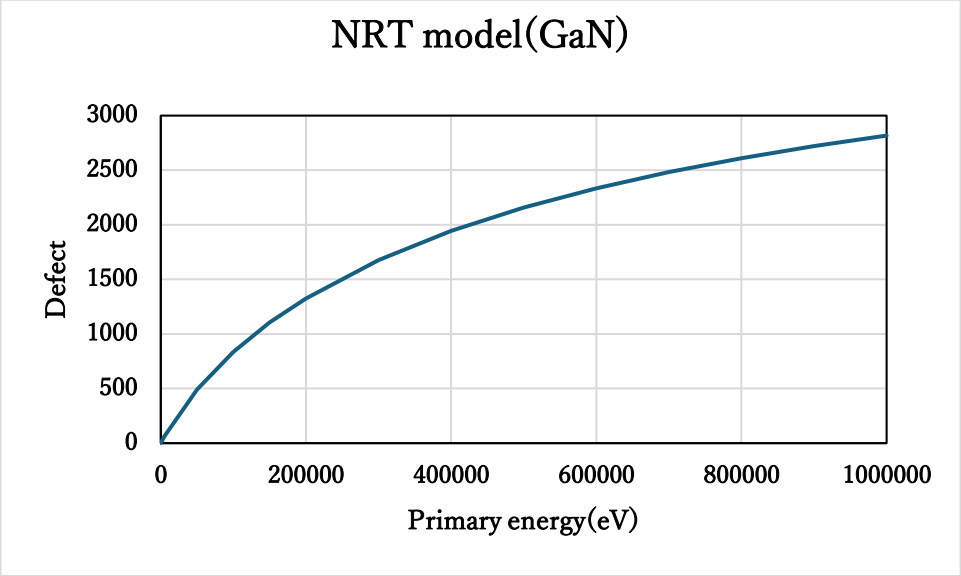
$$k = 0.1337\ Z_1^{1/6}\ \left(\frac{Z_1}{A_1}\right)^{0.5}$$

$$\varepsilon = \frac{A_2\ E_p}{(A_1 + A_2)} \frac{a}{Z_1\ Z_2\ e^2}$$

$$g(\varepsilon) = 3.4008\ \varepsilon^{1/6} + 0.40244\ \varepsilon^{3/4} + \varepsilon$$

$$a = \left(\frac{9\ \pi^2}{128}\right)^{1/3} a_0 \left(Z_1^{2/3} + Z_2^{2/3}\right)^{-0.5}$$

Here, Ep is the incident ion energy, Ed is the displacement energy, Z1 A1 is the incident ion atomic number and mass number, Z2 A2 is the target atomic number and mass number, and a0 is the Bohr radius. The results of calculating the Frenkel pairs generated when GaN is irradiated with Mg ions based on this formula are shown in the figure below.



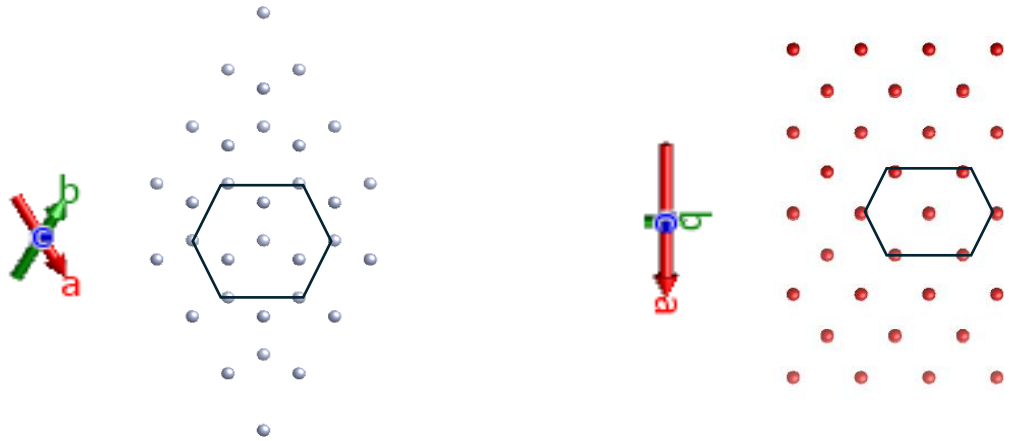
According to this NRT model, the defect generation rate when the incident energy is 180 keV is about 1000 per ion. If 10 incident ions are generated, the number of defects will be 10,000, and all of this data must be stored. If 30 incident ions are generated, more than 30,000 pieces of data must be stored in one irradiation process. The maximum number of defect data that MARLOWE can store is 32767. Therefore, if more than 30 incident ions are set, an error called storage overflow may occur. This was the cause of errors when calculating damage accumulation using MARLOWE. To avoid this, it is necessary to limit the number of incident ions, which is determined by the dose and implantation area. However, in order to perform a realistic analysis, it is necessary to keep in mind that the damage accumulation is underestimated.

Crystal compatibility of gallium oxide and gallium nitride

GaN crystal structure is hexagonal, with the a-axis and b-axis at 3.18 Å, the c-axis at 5.18 Å, and the angle β between the a-axis, b-axis and c-axis at 90 degrees. β-type Ga2O3 crystal structure is monoclinic, with the a-axis at 12.22 Å, the b-axis at 3.04 Å, the c-axis at 5.81 Å, and the angle β between the a-axis and c-axis at 103.82 degrees. Assume that a thin film of gallium oxide is formed on gallium nitride. The β-type gallium oxide that matches the (0001) plane of gallium nitride is the (-201) plane [9].

The relationship of the crystal orientation is as shown in the diagram below. The left side shows the nitrogen arrangement on the gallium nitride (0001) surface. The right side shows the oxygen arrangement on the beta-type gallium oxide (-201) surface.

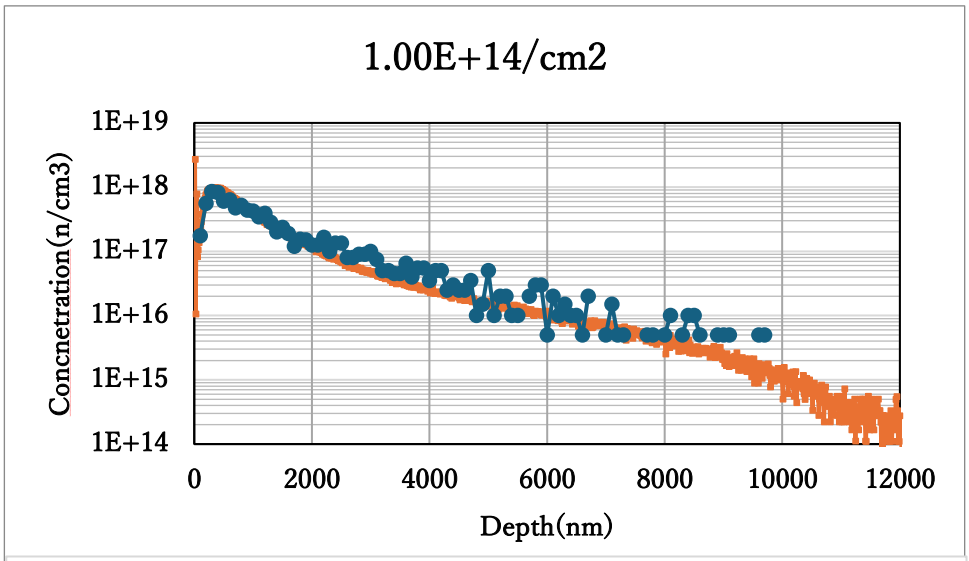
From this diagram, the b-axis [010] direction of gallium oxide coincides with the [11-20] direction of GaN. In other words, the (11-20) surface of GaN matches the (010) surface of Ga2O3. The lattice spacing of the GaN (2-200) surface is 1.38Å, while the lattice spacing of the Ga2O3 (020) surface is 1.52Å. The lattice mismatch is 10%.

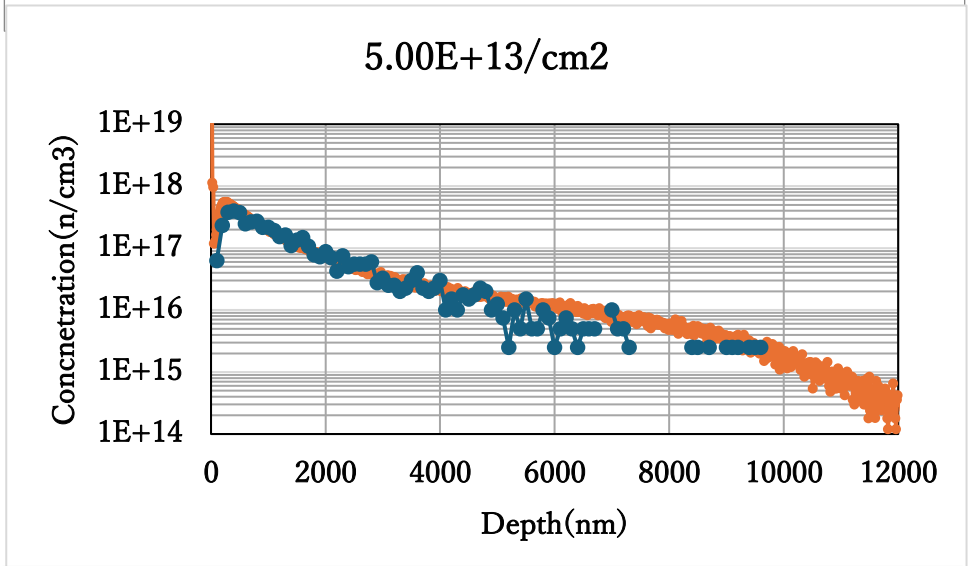


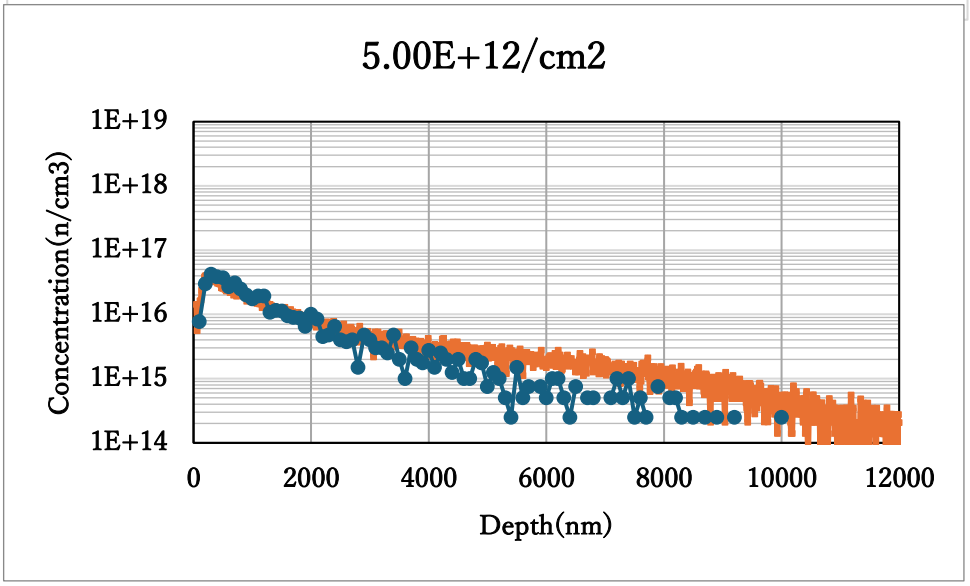
The Mg profile for 180 keV Mg channeling implantation with a surface gallium oxide film thickness of 10 Å will be presented in the next section.

Dose dependence of channeling profile

We analyzed how the channeling profile changes with dose.

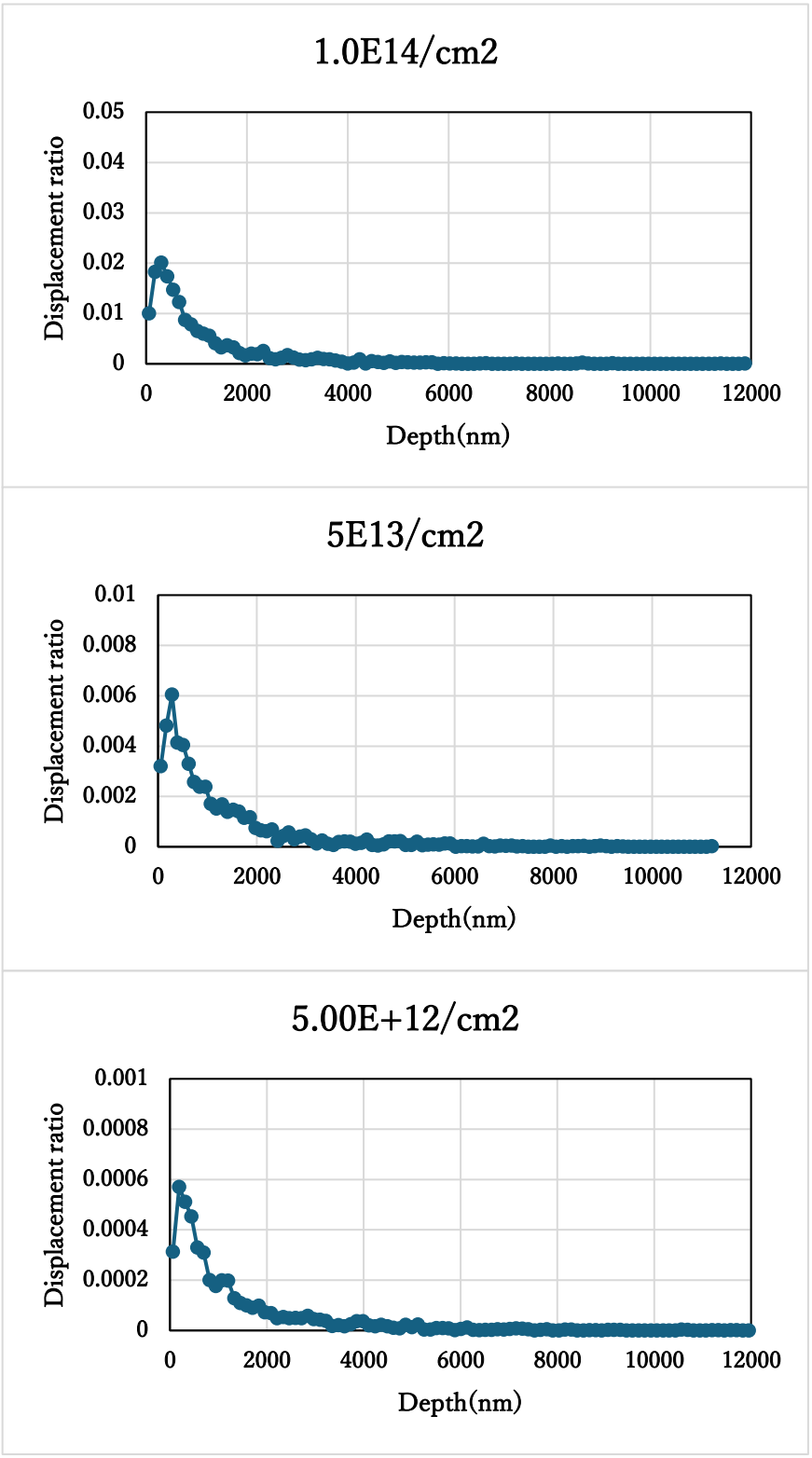






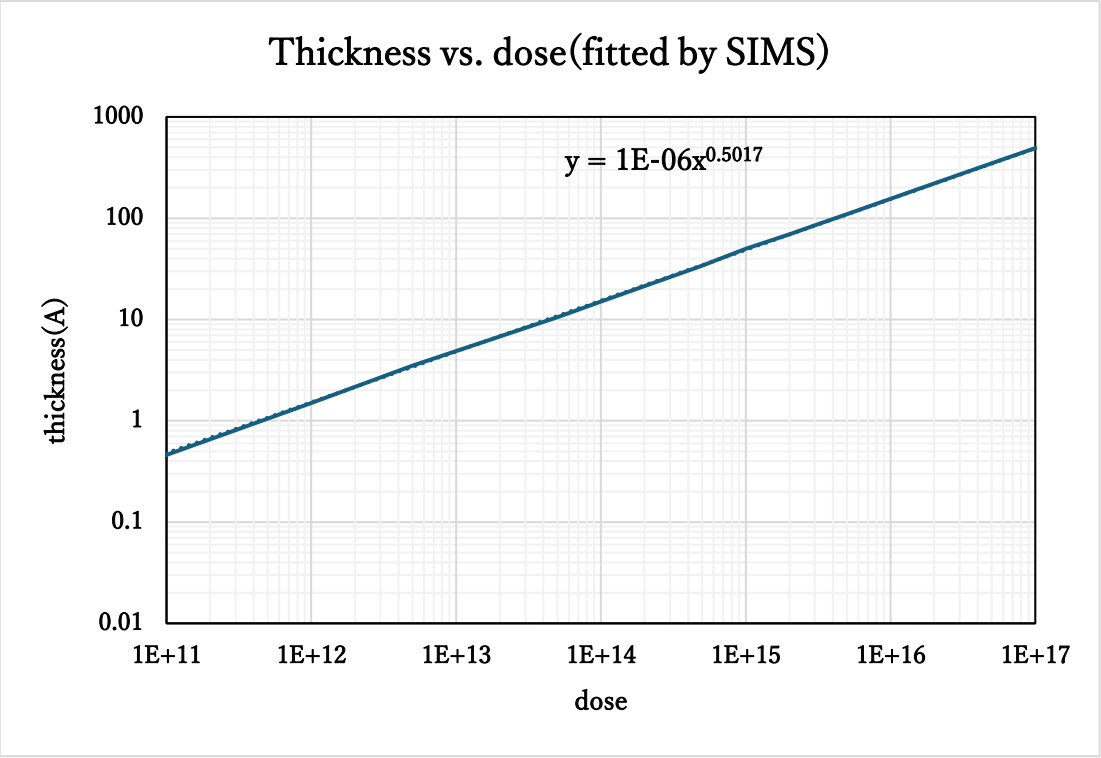
Dose Dependence of Damage

The depth distribution of Frenkel pairs formed by ion scattering was analyzed. The ratio of the number of Frenkel pairs generated to the atomic density of the substrate was calculated. Since the damage caused by channeling implantation is very small and difficult to detect by RBS, it is necessary to perform highly sensitive strain analysis using X-ray rocking curves.

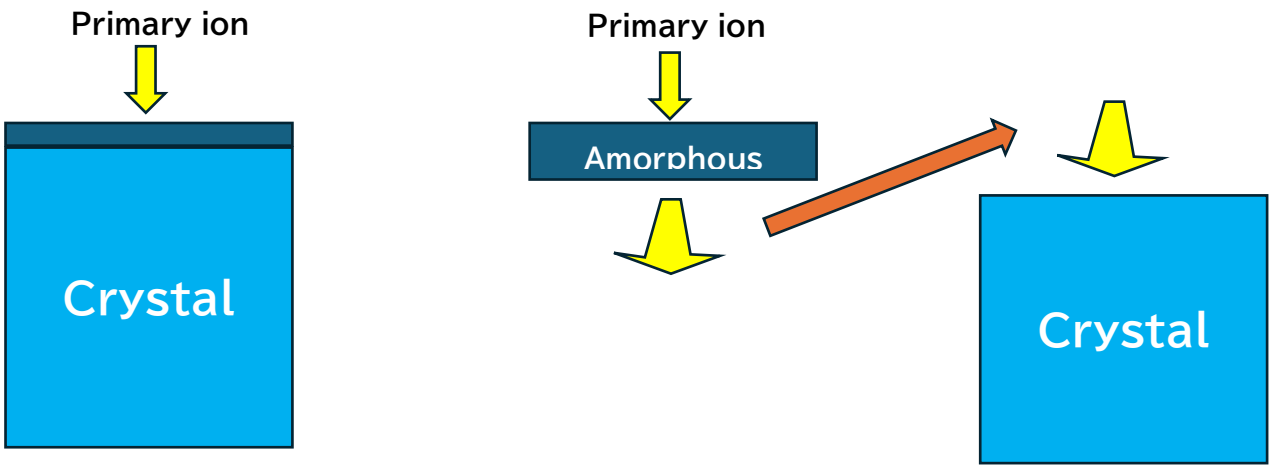


Effect of amorphous films to primary ion

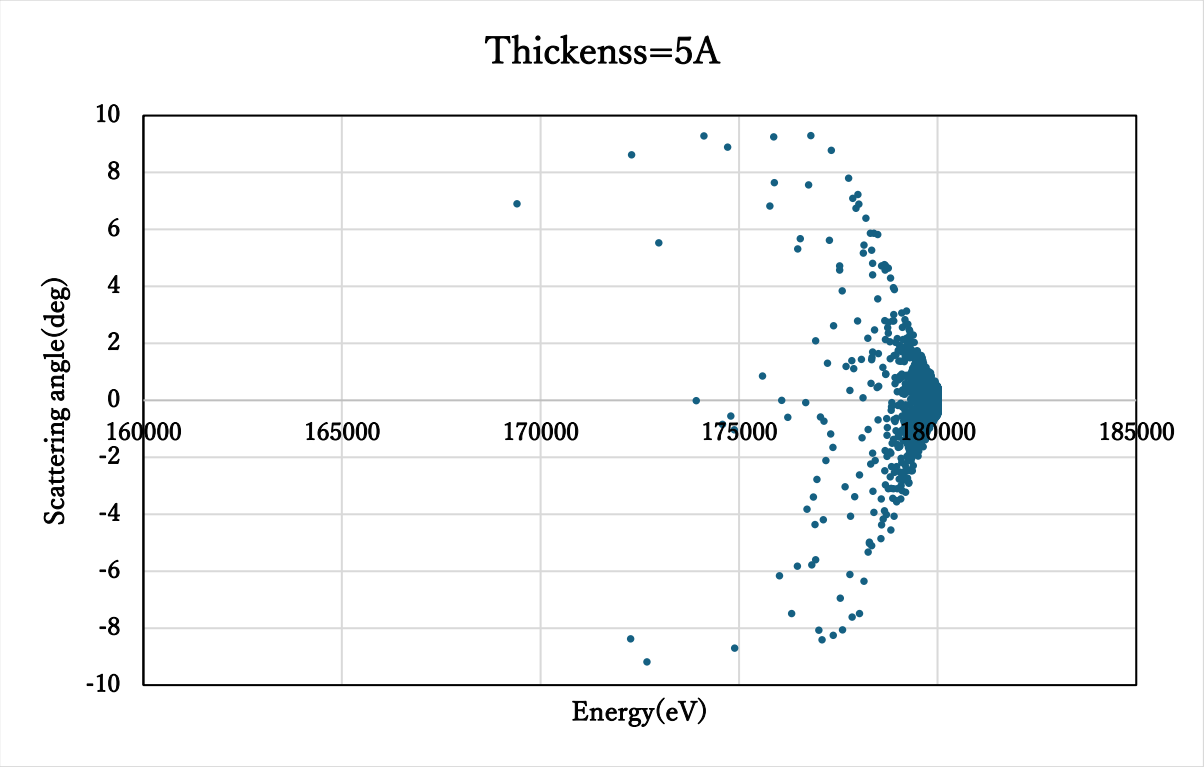
Our analysis so far has confirmed that SIMS profiles can be reproduced by adjusting the virtually set amorphous film thickness [6]. Since the adjusted amorphous film thickness is about 15 Å even at 1E14/cm2, it is clear that a very thin amorphous layer affects the channeling profile. Furthermore, as shown in the graph, it has been found that the amorphous film thickness is proportional to the square root of the dose.



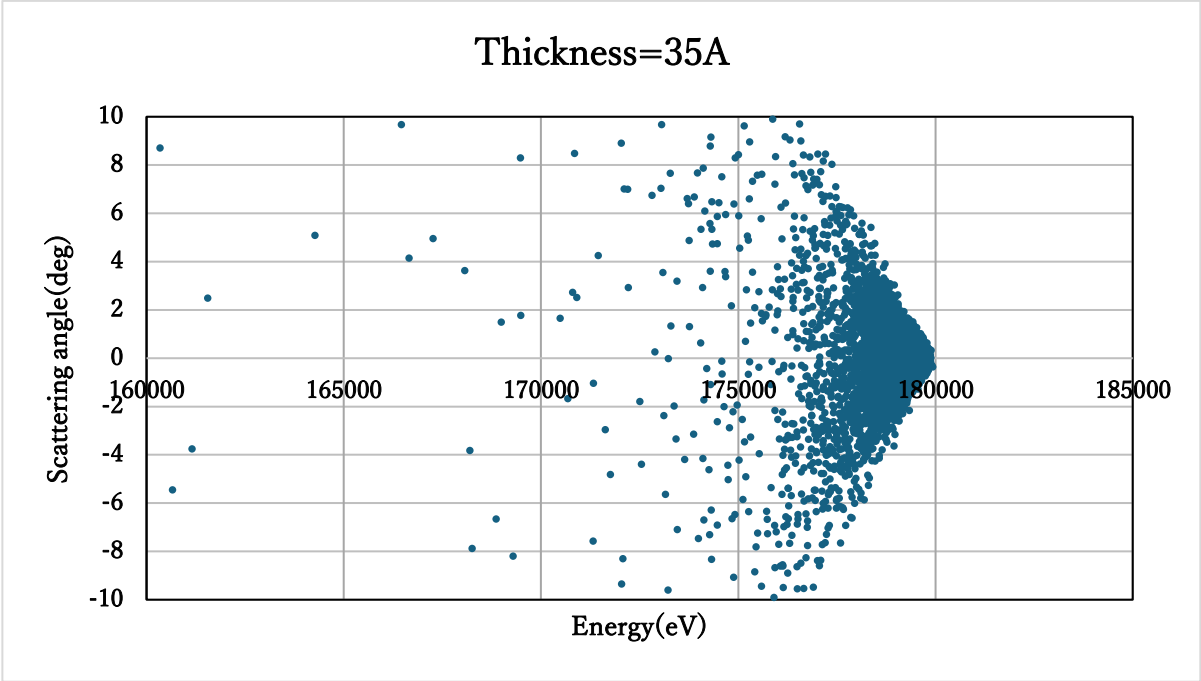
Therefore, we analyzed how the incident ions are scattered by this amorphous layer. The divergence angle of the incident ions is set at 0.5 degree. We investigated how the energy and scattering angle of primary ion will be affected through the amorphous layer.



The next graphs show the correlation between energy and scattering angle of primary ion after passing through amorphous layer. The thickness of amorphous layer is 5 Å and 35 Å. As the energy of primary ion is 180keV, the energy is distributed below 180keV. And as the scattering angle becomes large, the energy of scattered primary ion decreases.



The decrease of energy of scattered primary ion energy becomes large, and the distribution of scattering angle becomes large.



Dose-square-root dependence of defect density

As a supplementary note, since it is generally known that the defect density caused by ion irradiation is proportional to the square root of the dose, we will introduce the basic concept [10]. It is known that the generation of interstitial atoms and vacancies due to irradiation can be analyzed using a chemical reaction equation. This basic equation is shown below.

$$\frac{dC_v}{dt} = G - K_{iv}\, C_i\, C_v - K_v\, C_v$$

$$\frac{dC_i}{dt} = G - K_{iv}\, C_v\, C_i - K_i\, C_i$$

Here, Cv and Ci are the vacancy and interstitial atomic densities, Kiv is the reaction constant between interstitial atoms and vacancies, and G is the generation rate of Frenkel pairs due to irradiation. Kv and Ki are the annihilation reaction constants due to the sink of point defects. If we calculate the steady state ignoring annihilation due to the sink, the vacancy and interstitial atom densities are as follows. Since G is proportional to the irradiation dose, the steady-state defect density is proportional to the square root of the dose.

$$C_i^{st} = C_v^{st} = \sqrt{\frac{G}{K_{iv}}}$$

On the other hand, if we consider a special situation in which interstitial atoms and vacancies do not react, the defect concentration is linearly proportional to the dose.

Summary

The damage accumulation model by MARLOWE enabled us to analyze the channeling profile caused by boron ion irradiation of silicon. As a result, it was confirmed that the dechanneling phenomenon caused by the generated interstitial atoms could be reproduced.

From the beginning of analysis using MARLOWE, there was a problem that errors occurred when the dose was high due to limitations specific to MARLOWE. However, it was confirmed by model calculations of Frenkel pair production that when a large number of Frenkel pairs are generated by ion collisions, the limit of data storage capacity is exceeded. At present, there are difficulties in utilizing the damage accumulation model in terms of analysis time and data capacity. However, it can provide basic information on damage evaluation.

We analyzed the channeling profile assuming the presence of a crystalline β-type gallium oxide thin film on the GaN surface, and confirmed that it corresponded to SIMS. However, it is not realistic to analyze the change in the channeling profile relative to the dose with high statistical accuracy. Therefore, we have performed a realistic analysis by setting a virtual amorphous film on the target surface. In this article, we have shown that it is possible to identify the scattering phenomenon that occurs by assuming an amorphous film.

References

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