Basic of critical angle for channeling ion implantation

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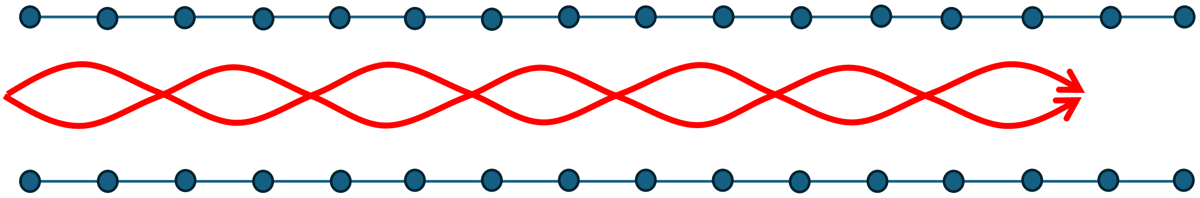
Introduction

For the past few years, I have been analyzing the phenomenon of channeling ion implantation using MARLOWE code, and have been working on matching the channeling profiles with SIMS profiles, mainly for compound semiconductors such as 4H-SiC and GaN.
This article explains the summary of the critical angle, a basic aspect of the channeling phenomenon.

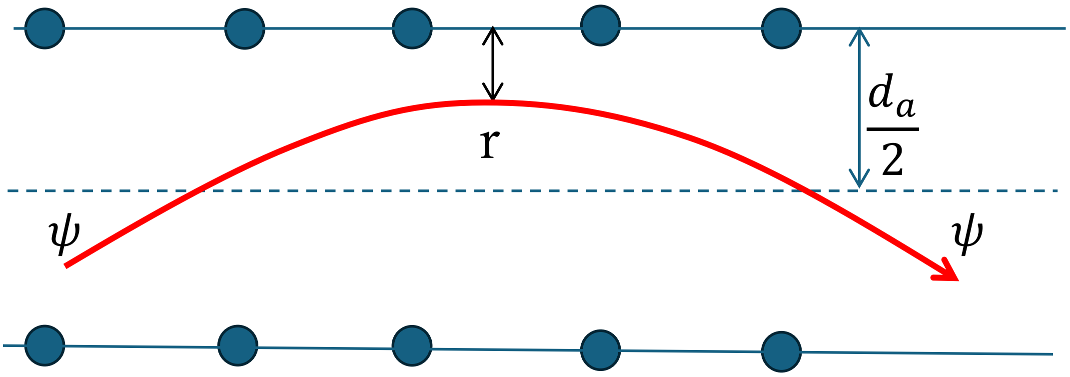
Let's briefly review the channeling phenomenon using the diagram below. When an ion enters the crystal axis at an angle close to parallel to the axis, it is captured by the potential around the crystal axis and proceeds, which is called channeling. Ideally, an ion that enters the crystal axis will penetrate very far. It is easy to expect that channeling is hindered when the angle of incidence to the crystal axis becomes larger.



It is well known that channeling is used to achieve deep implantation into semiconductors. However, in the field of elementary particle physics, a technology has been developed to pass an ultra-high energy beam of the GeV order through a curved crystal and deflect it, where the channeling phenomenon is also applied, and detailed analysis has been carried out to propose a practical model. In this article, I have explained the concept of the critical angle related to the channeling phenomenon as much as possible with diagrams and kept the mathematical formulas to a minimum, so I hope that reading through to the end will help you understand.

Definition of critical angle

In channeling implantation, ions must be incident along the crystal axis of the target. However, channeling is inhibited by the inclination of the incident angle, and a critical angle is defined to evaluate how much inclination of the incident angle is tolerated.



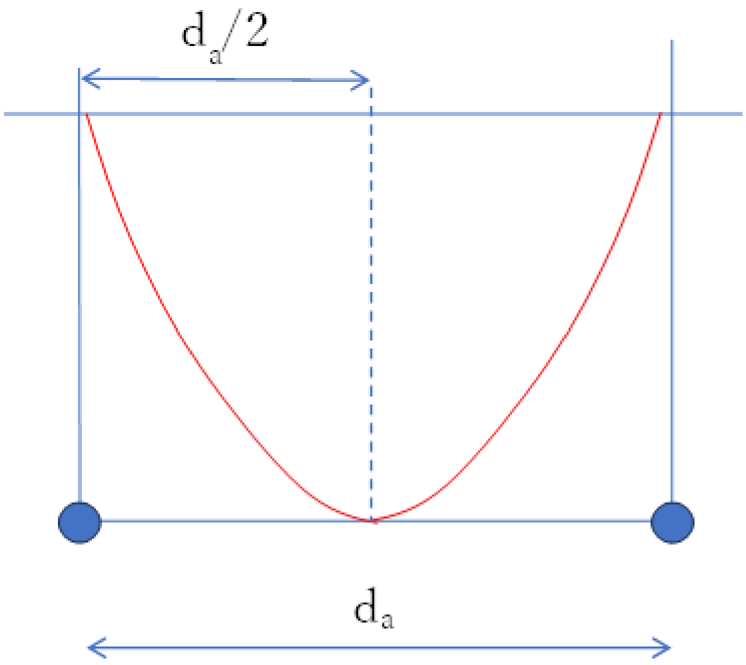
From the schematic diagram of the channeling phenomenon, an ion incident at an angle of ψ along the crystal axis is reflected by the potential of the crystal axis at position r. At this position, the kinetic energy of the ion in the direction perpendicular to the direction of travel is zero. However, the kinetic energy in the perpendicular direction at any position is as follows:

$$E\ sin^2\psi$$

In the case of channeling implantation, the angle of incidence is small, so a sine function approximation can be applied. Furthermore, the conservation law of the sum of kinetic energy and potential energy gives the following equation for the ion's traveling direction and the perpendicular direction. The minimum value of the potential energy is defined as the midpoint of the crystal axis.

$$E_\perp = U(r) = E\,\psi^2 + U\left(\frac{d_a}{2}\right)$$

A schematic diagram of the potential felt by an incident ion is shown below. The potential seen from the direction of ion movement increases as the ion approaches the crystal axis.



When the incident angle of the ions is increased, they reach the closest position (rc) to the crystal axis. This incident angle is defined as the maximum angle (ψmax) at which channeling occurs.

$$E_{\perp} = U(r_c) = E\,\psi_{max}^2 + U\left(\frac{d_a}{2}\right)$$

From the potential distribution diagram, the potential energy satisfies the following relationship.

$$U(r) < U(r_c)$$

If ions are incident at an angle equal to or greater than the maximum angle at which channeling occurs, channeling will be inhibited. Therefore, the critical angle can be calculated as follows:

$$\psi_{max} = \sqrt{\frac{U(r_c) - U\left(\frac{d_a}{2}\right)}{E}}$$

Inter-atomic potential

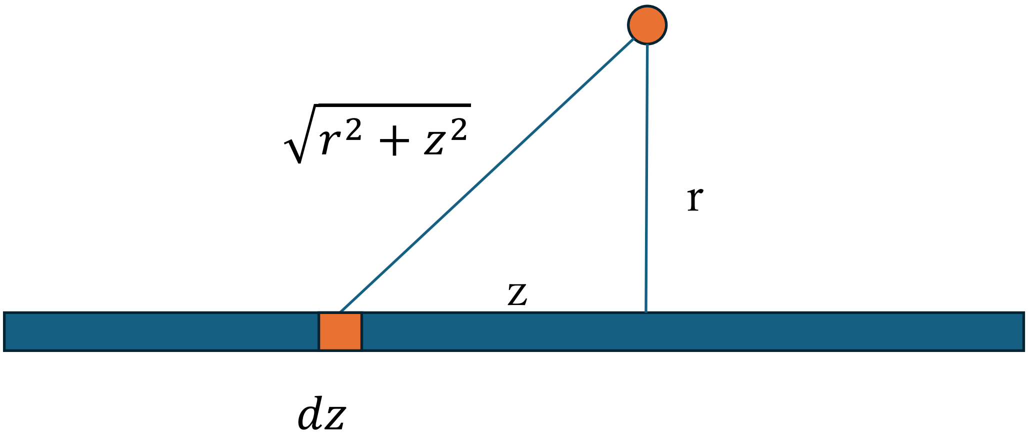
Next, we calculate the potential felt by the ion. The inter-atomic potential is generally expressed by the following formula. Here, Z1 represents the atomic number of the incident ion, Z2 represents the atomic number of the target atom, and r represents the distance between the incident ion and the target atom. The function g is defined as a screening function and differs depending on the shape of the potential. Furthermore, several expressions have been proposed for the parameter a as the screening length, but it is basically a function of the atomic numbers of the incident ion and the target atom.

$$U(r) = \frac{Z_1 Z_2 e^2}{4\pi\varepsilon_0 r} g\left(\frac{r}{a}\right)$$

$$a \propto \frac{a_0}{\sqrt{Z_1^{2/3} + Z_2^{2/3}}}$$

$$g(r) = \sum_1^3 \alpha_i \, exp\left(\frac{r\,\beta_i}{a}\right)$$

The average potential felt by the incident ion is calculated by the sum of the potentials from each atom that is a distance r away. If we assume that the crystal axis is a continuum of electric charge and that the electric charge is uniformly distributed over the atomic distance d, the arrangement of the electric charge and the incident ion at dz is as shown in the figure below.



The continuum potential can be calculated by integrating the crystal axes from -∞ to ∞ as follows:

$$U_{ax}(r) = \frac{1}{d}\int_{-\frac{d}{2}}^{\frac{d}{2}} dz \sum_{j=-\infty}^{j=\infty} U\left(\sqrt{r^2 + (z - j\,d)^2}\right) = \frac{1}{d}\int_{-\infty}^{\infty} U\left(\sqrt{r^2 + z^2}\right) dz$$

By analytically solving the integral of this equation, we can express it as the following equation.

$$U_{ax}(r) = \frac{2\,Z_1\,Z_2\,e^2}{4\pi\varepsilon_0\,d} f\left(\frac{r}{a}\right)$$

$$f(\xi) = \sum_{i=1}^{3} \alpha_i\,K_0(\beta_i\,\xi)$$

The function K_0 is the zeroth-order Bessel function.

Minimum distance of approach

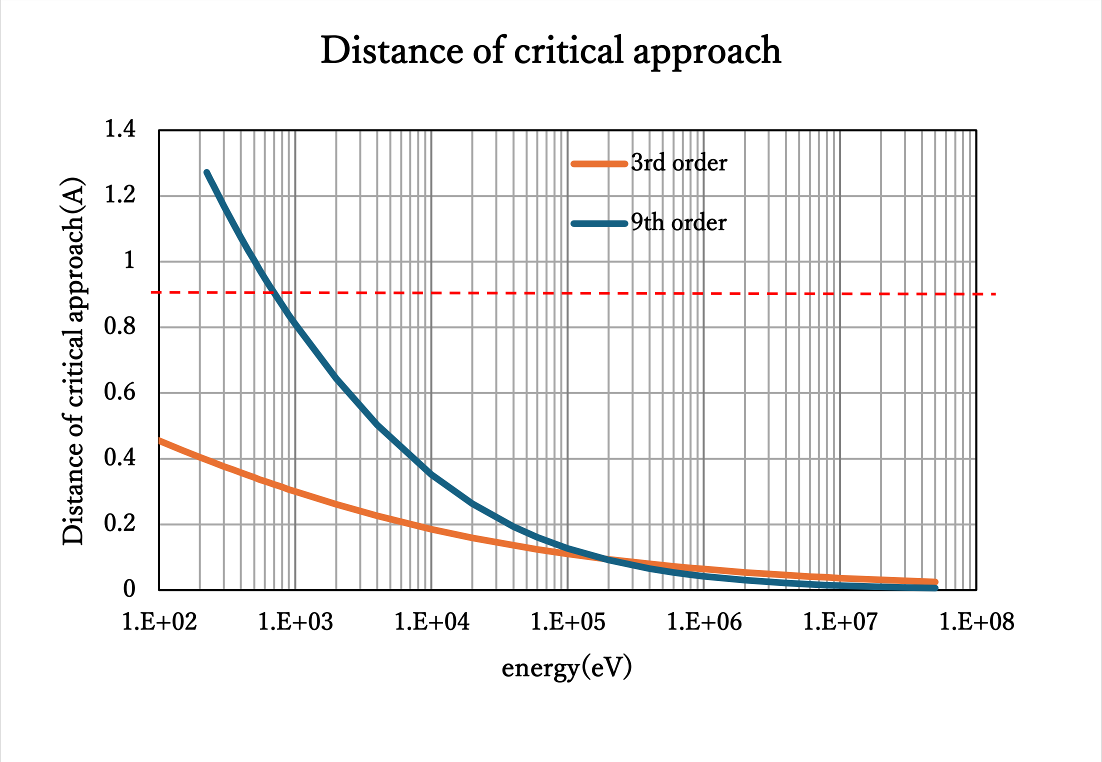
Next, we will explain the nearest approach distance. To calculate the nearest approach distance, a third-order approximation formula was proposed using the square root of the parameter α, which is proportional to the reciprocal of the incident energy E.

$$r_c = \frac{2}{3}\,a\,\sqrt{\alpha}\left[1 - \frac{\sqrt{\alpha}}{19} + \frac{\alpha}{700}\right]$$

$$\alpha = \frac{Z_1\,Z_2\,e^2\,d}{4\pi\varepsilon_0\,a^2 E}$$

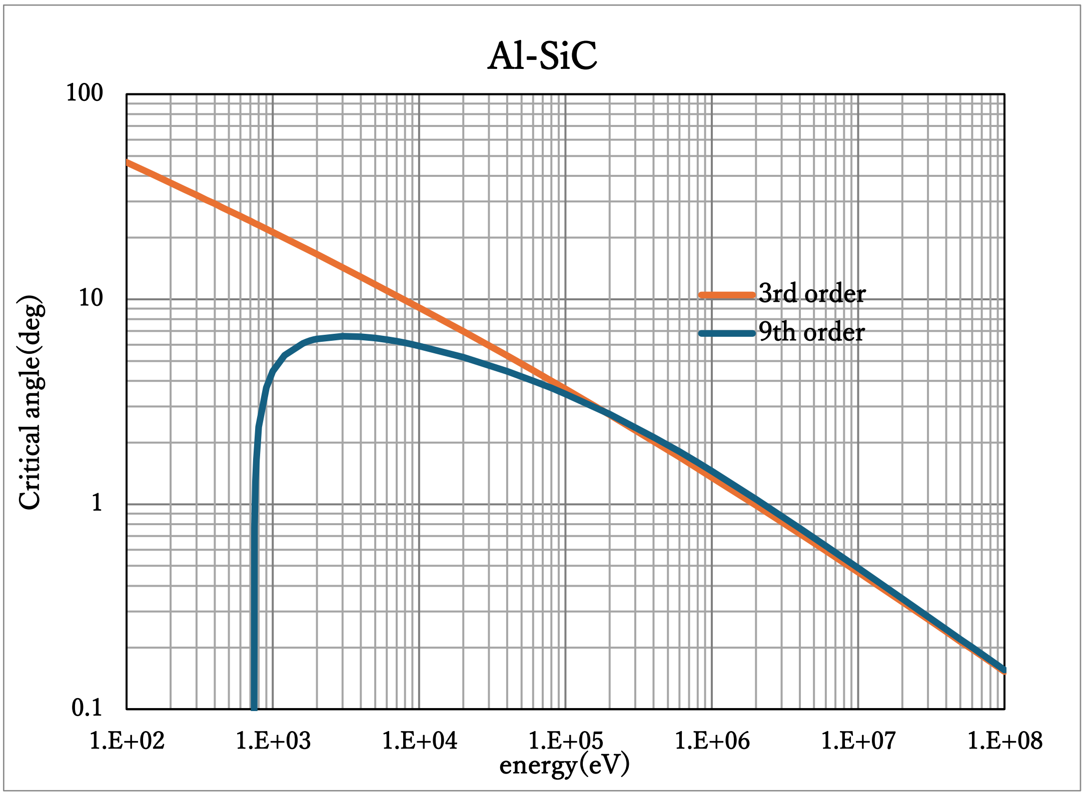
However, it is known that the third-order approximation formula has limitations in handling the low energy region. In order to analyze the channeling phenomenon in detail over a wide energy range, it has become possible to express it as a ninth-order approximation formula of the square root of α, which allows for more accurate analysis.

The following figure shows the incidence energy dependence of the nearest neighbor distance when channeling Al into 4H-SiC. In the third and ninth order approximations, we can see that the nearest neighbor distances deviate significantly in the energy region below 100 keV. In the case of 4H-SiC, da/2 is 0.89 Å based on the crystal structure. Therefore, when the incidence energy is 700 eV or less, the nearest neighbor distance becomes larger than 0.89 Å, and channeling is hindered.



Critical angle

Based on the definition of the critical angle, we obtained the energy dependence of the critical angle when Al is implanted into 4H-SiC by channeling. The critical angle below 100 keV is dissociated due to the difference between the third and ninth order approximations of the nearest neighbor distance. Furthermore, it is found that 700 eV is the minimum energy at which channeling is possible. This tendency is also clear from the explanation using the ninth order approximation of the nearest neighbor distance. The definition of critical angle was the angle that a primary ion closes to a axial potential wall. That is to say, a critical angle is the situation that the channeling condition changes to the random condition.



Appendix

For targets consisting of a single atom, the formula is easy to handle. However, for compounds, there are several things to consider.

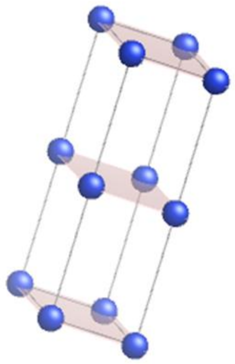
One of them is how to define the atomic number of the target. Usually, for two atoms, the average of the atomic numbers is used. This assumption has been shown to be valid from the potential distribution.

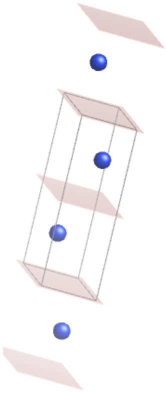
$$Z_{SiC} = \frac{Z_{Si} + Z_C}{2}$$

The second is the definition of the screening parameters. For example, in the case of SiC, the screening parameters of Al and Si and the screening parameters of Al and C can be calculated and averaged.

$$a_{Al-SiC} = \frac{a_{Al-Si} + a_{Al-C}}{2}$$

The third is the definition of the interatomic distance along the crystal axis. In the case of silicon, the lattice constant a can be applied. However, in the case of hexagonal crystals such as 4H-SiC, it is necessary to calculate the average interatomic distance. As can be seen from the figure below, the interatomic distance along the crystal axis can be c/2 or c.





The fourth step is to find the position of the minimum potential. For example, in the case of silicon <100> incidence, the position a/4 from the atomic position is the minimum potential, as shown in the figure below.