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Channeling energy loss and dechanneling of He along axial and planar directions of Si

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ABSTRACT

In the present work, the energy loss and the dechanneling of He ions in the energy of 1.5 MeV and 2 MeV along the ⟨100⟩ and ⟨110⟩ axial directions as well as the {100} and {110} planar directions of Si were studied by the simulation of the channeling Rutherford backscattering spectra. The simulation was done based on the considerations that a fraction of the aligned beam enters the sample as a random component due to the ions scattering from the surface, and the dechanneling starts at the greater penetration depths, x_{Dech}. It was presumed that the dechanneling process follows a simple exponential law with a parameter λ which is proportional to the half-thickness. The Levenberg–Marquardt algorithm was used to set the best parameters of energy loss ratio, x_{Dech} and λ. The experimental results are well reproduced by this simulation. Differences between various axial and planar channels in the Si crystal and their influence on the energy loss ratio and dechanneling of He ions are described. Moreover, the energy dependence of energy loss ratio and dechanneling of He ions were investigated. It is shown that the dechanneling behavior of ions depends on the energy and energy loss of the ions along a channel. The channeled to random energy loss increases by decreasing ions energy.

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1. Introduction

Since the discovery of channeling phenomenon, the problems of the channeling energy loss and the dechanneling of ions have been concerned.

It was observed that the energy loss of ions along the low index axis or plane of crystal is a fraction of their random energy loss due to less electron density along the channel. Then the necessity of the precise knowledge of the channeling energy loss for depth profiling of elements in the matter led to an extensively study of the energy loss for different sorts of ions and crystals [1–4].

Besides, by the dechanneling of ions we can acquire information about the interaction of ions with lattice atoms and about the kind and the amount of crystal imperfections. The knowledge of the dechanneling is important for both fundamental physics studies and its application. So several experiments have been devoted to the investigation of the critical angle and aligned minimum yield to understand the dechanneling process [5–7]. Some research papers were theoretically studied the dechanneling of ions by means of Lindhard diffusion model by Bonderup et al. [8], Ga et al. [9], Burenkov et al. [10] and, Morita and Itoh [11]. Kitagawa and Ohtsuki derived a modified diffusion equation from the Fokker–Planck equation and calculated the dechanneling range for 1.5 MeV protons, deuterons and alpha in the Ge ⟨100⟩ axis [12]. Altman et al. studied the temperature dependence of the dechanneling length, at which the numbers of channeled ions reduce to half, for 5 MeV transmitted protons along the {110} and {111} planes of Si [13]. The dechanneling rate and range of protons in the energy range of 1–10 MeV along the axial channels of Si were calculated theoretically by Petrović et al. [14]. The dechanneling parameters of deuteron and its channeling energy loss along different axial and planar channels of Si were recently calculated by simulation of RBS/C spectra [15]. Overall, the majority of papers revolve around the dechanneling of ions specially protons, theoretically. Some papers just considered the minimum yield of ions penetrating into the channel by means of experimental method [5,7]. There is not an entire document concerning the parameters to explain the dechanneling of He along various channels of crystals.

In this paper, the channeling energy loss and the dechanneling of 1.5 MeV and 2 MeV He ions along the ⟨100⟩ and ⟨110⟩ axial directions and the {100} and {110} planar directions of Si were studied by simulation of the RBS/C spectra. A silicon wafer cut normal to the plane (100) was used as a sample. It was assumed that the dechanneling process follows the simple exponential function

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with a parameter λ, which is proportional to the half-thickness $x_{1/2}$, presenting the distance at which the numbers of ions reduce to half. The dechanneling was considered to start at the greater penetration depths x_{Dech}. In addition, the minimum random component of the channeled ion beam entering the sample due to ion scattering from the surface rows of atoms was involved in the simulation. The ratio of channeling to random energy loss, λ and x_{Dech} were deduced by adapting the experimental and the simulation results with each other utilizing the Levenberg–Marquart algorithm. The dechanneling process of He ions was described by two parameters x_{Dech} and $x_{1/2}$. The same target and laboratory conditions to take all the axial and planar spectra, enabled us to compare the dechanneling process of He in the ⟨1 0 0⟩ and ⟨1 1 0⟩ axial and the {1 0 0} and {1 1 0} planar directions to get more information about the influence of the crystal configuration on the channeled ion trajectory. The energy dependence of the dechanneling parameters was also studied. The ratio of channeling to random energy loss along the axial and planar channels was obtained and compared with the other reference. The consistency between values confirms our method and obtained values. This method can also be used for studying the dechanneling parameters of He in other targets.

2. Experimental procedure

The Si crystal wafer cut in the direction of the plane (1 0 0) was cleaned and etched by using 10% HF just before the RBS measurements and used as a target. The sample was mounted on a 3-axes goniometer with an accuracy of 0.01° which allowed aligning the incident beam with different planar and axial directions of the target. The appropriate slits limit the divergence angle of the beam less than 0.06°. The Si surface barrier detector was employed at the angle $\theta = 165°$ with respect to the incident beam. The energy resolution of the detection system was 15 keV. The ion beams with different energies were produced by a 3 MeV Van de Graaff accelerator.

The {1 0 0} and {1 1 0} planar directions were determined by an angular scan of the target. Then, the beam was aligned to the ⟨1 0 0⟩ axis of the crystal by following the planar channels trance by tilting the target in 0.4° steps gradually. It was observed that the three planar directions approach one another and finally the ⟨1 0 0⟩ axis position was revealed. The ⟨1 1 0⟩ channel was obtained in the similar way of the ⟨1 0 0⟩ channel after turning the angular position of the sample by 45°. The spectrum of each direction was taken in the energy 1.5 MeV and 2 MeV in the tilt angle at which the backscattering particles count was the minimum. Random spectra were taken by 3° away from the axial and the planar directions. A χ_{min} of about 3% showed the good quality of the target.

3. Principle method

The method used for the simulation of the channeling Rutherford backscattering spectra has recently been described [16]. The simulation program was written in standard language C++. The target was divided into slices of thickness $dx = 30$ Å.

It is known that the probability of the ions collision with the sample surface atoms is independent of the incident ions alignment; though, the backscattered ions yield reduces on the target surface in the channeling spectrum compared to the random one due to the energy and depth resolution limitation of the detector system. Then, at first few atom layers, the shadowing effect rapidly decreases the interaction yield and a surface peak appears. As a result, a fraction of the ion beam branches off from the channeled beam and enters the target as a random component. The minimum yield corresponding to the minimum random component takes place immediately after the surface peak [17].

Thus, in the simulation, the beam was split into two parts: a random part and a channeled part. The simulation of the surface peak was ignored, because it gives no information about the channeling and the dechanneling of the ions. But the minimum random component of the beam entering the target contributes to the rest of backscattered ions yield so it was considered as a consequence of the collisions of the ions with the target surface and the first few atomic layers. The initial random portion of ion beam can be determined by two methods. First, it is determined from the minimum of normalized angular yield about each channel. In the second method, it can be calculated from the normalized yield immediately behind the surface peak (in the axial case) or near the edge of spectrum (in the planar case). The second method was utilized in this paper.

For the random part of the beam, as regards the amount of χ_{min} measured from the channeling experimental spectrum, the backscattering probability ions in each slice were evaluated. Then the energy of ions when they exit the sample was calculated by:

$$E_{\text{R-out}} = \left[K\left(E_0 - \int_0^{x_R}(dE/dx)dx\right)\right] - \int_0^{x_R/\cos\theta}(dE/dx)dx \tag{1}$$

where K is the kinematic factor and x_R is the distance the ions passed in the target.

The channeled part of the ion beam keeps penetrating through the channel until it gets adequate transverse energy to escape from the channel. This increases the backscattered ion yield from the minimum yield. The depth, x_{Dech}, at which the dechanneling starts, was deduced by the simulation of the channeling spectra. It was assumed that the dechanneling follows an exponential pattern given by Aslanoglou et al. [2]:

$$N_d = N_0(1 - e^{-x/\lambda}) \tag{2}$$

where N_0 is the number of ions initially in the channel, and λ is an energy independent parameter. The number of ions escaping from the channel at a depth between x and $x + dx$ is expressed by:

$$dN_d = (N_0/\lambda)e^{-x/\lambda}dx \tag{3}$$

The depth at which the numbers of the ions reduce to half is indicated by half-thickness obtained by:

$$x_{1/2} = \lambda \ln 2 \tag{4}$$

In each slice the number of the dechanneled ions and their energies were evaluated. It is worth mentioning that the channeled particles suffer only a portion energy loss of random one:

$$(dE/dx)_{\text{Channel}} = \alpha(dE/dx)_{\text{Random}} \quad 0 < \alpha < 1 \tag{5}$$

where α is also assumed to be energy independent. The part of the beam which had been dechanneled was considered as the random one. Therefore, its stopping power was calculated with the Ziegler formula and approximation [18]. The energy of these ions when left the target in regard to the backscattering in each latter slice was calculated by:

$$E_{\text{out}} = K\left[E_0 - \left(\int_0^{x_{ch}} \alpha\left(\frac{dE}{dx}\right)dx + \int_0^{x_R}\left(\frac{dE}{dx}\right)dx\right)\right] - \int_0^{x_{ch}+x_R/\cos\theta}\left(\frac{dE}{dx}\right)dx \tag{6}$$

where x_{ch} is the distance the ions had passed through the channel before being dechanneled.

The number of backscattered ions is given by:

$$N_{\text{det}} = N_{\text{inc}} \times \left(\frac{d\sigma}{d\Omega}\right) \times N_{\text{target}} \times \Delta\Omega \tag{7}$$

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