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Dechanneling and the energy loss of protons along planar directions of Si

Sepideh Shafiei*, Mohammad Lamehi-Rachti

Physics and Accelerators Research School, Nuclear Science and Technology Research Institute, AEOI, P.O. Box: 113653486, Tehran, Iran

HIGHLIGHTS

- The RBS/C spectrum of 1400-2200 keV protons along the planar direction of Si was taken and analyzed
- A simulation method was proposed to determine the dechanneling and the energy loss parameters.
- The simulation was done based on the basic concept of the channeling phenomena.
- The dechanneling process was clearly explained by the exponential function.

ABSTRACT

In the present paper, the dechanneling and the energy loss of protons at the energy interval of 1400 to 2200 keV along the {100} and the {110} planar directions of Si were studied by the simulation of the measured channeling Rutherford back-scattering spectra based on the exponential dechanneling function with a parameter λ. This parameter is proportional to the dechanneling rate and represents the mean distance that ions travel along the channel before escaping from the channel. The Levenberg-Marquardt algorithm was used to set the best values of the channeling to random energy loss ratio, and the mean channeling distance. The experimental results are well reproduced by this simulation. The data analyzed in this energy range did not show any particular trend with regard to energy dependence of the parameters. The differences between both the planar channels in the Si crystal and their influence on the energy loss ratio and dechanneling of proton ions are described.

KEYWORDS

Backscattering Spectrometry
Proton ions
Channeling stopping power
Mean channeling distance

HISTORY

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1 Introduction

Since the early days of ion channeling discovery, the electronic distribution and the ion-atom interaction along the low-index axes and planes of crystalline materials have been studied. The interpretation of the channeling phenomenon was done by investigating the channeling energy loss and the dechanneling parameters by experimental, computational and theoretical methods.

When ions enter the channel of a crystal, the atomic potential confines them in the middle of the channel far from the lattice atoms (Bird and Williams, 1989). Besides, the electron density along the channel is less than that in the random direction. Therefore, in the channel directions, the number of close impact-type collisions decreases. Subsequently, ions along the low index axis or plane of a crystal lose their energy, lower than the one in the random direction. The channeling energy loss information is important for studying the depth profiling of crystal structure, lattice damage (Feldman et al., 2012), lattice recovery by annealing (Eriksson et al., 1969), ion implantation (Mayer et al., 1968), and surface amorphous layer. So many papers have been devoted to this issue.

The sample that has been extensively studied is Si. The channeling stopping powers of medium and heavy-mass ions in Si was calculated (Azevedo et al., 2002; Eisen, 1968; Jiang et al., 1999; Bentini et al., 1991).

The channeling stopping power of the He ions with different energy in Si (Azevedo et al., 2002; Jarvis et al., 1977; Shao et al., 2006), Au (Robinson, 1971), InP (Hetherington, 1996), Ge (Culbertson et al., 1984) was studied. The limited research was down on measuring the channeling energy loss of deuteron in Si channels (Sattler and Dearnaley, 1967; Jarvis et al., 1979; Erramli et al., 2000; Valdés et al., 2000).

The channeling stopping power of protons in the various energies along the main axes (Lenkeit et al., 1990; Dettmann and Robinson, 1974; Kokkoris et al., 2003;

*Corresponding author: sshafiei@aeoi.org.ir

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Aslanoglou et al., 1998, 2000) and planes (Gehrmann et al., 1985; Vos et al., 1988) of Si target was measured.

Although there are a lot of data on the channeling stopping power of ions in the various samples, research on this topic has been done to obtain more precise values. Moreover, looking at the literature reveals the lack of channeling stopping power measurement along the planar directions.

Additionally, the dechanneling of the ions along the various channels of the target has been explored by means of the critical angle, the minimum yield (Derry et al., 1981; Roosendaal et al., 1974) and dechanneling parameters attained directly from the dechanneling function. Using the phenomenological approach for simulating the RBS/C spectrum based on the exponential or the Gompertz type dechanneling function leads to obtaining parameters such as the mean channeling distance or the dechanneling rate and range.

The dechanneling parameters of the proton ions along the low-index axes of Si have been investigated (Aslanoglou et al., 1998, 2000; Petrović et al., 2007; Kokkoris et al., 2003; Shafiei and Lamehi-Rashti, 2015). Though, the dechanneling of protons along the planar direction of Si has not been studied yet.

In the present article, the mean channeling distance of protons along the {100} and the {110} planar directions of Si as well as the ratio of channeling to random stopping power were presented. The parameters were calculated by the simulation of channeling Rutherford back-scattering spectra of protons in the energy interval of 1400 to 2200 keV along the {100} and the {110} planes of Si. It was assumed that the dechanneling process follows the simple exponential function. Using the same silicon wafer and laboratory conditions to take all the spectra makes the result comparable along the different channels. There was not any data for the parameter of λ, but the validity of the channeling stopping power showed that the simulations were done correctly. Since the values of these two parameters are somehow related to each other, the validity of the values of shows the validity of the calculated values of λ in this paper.

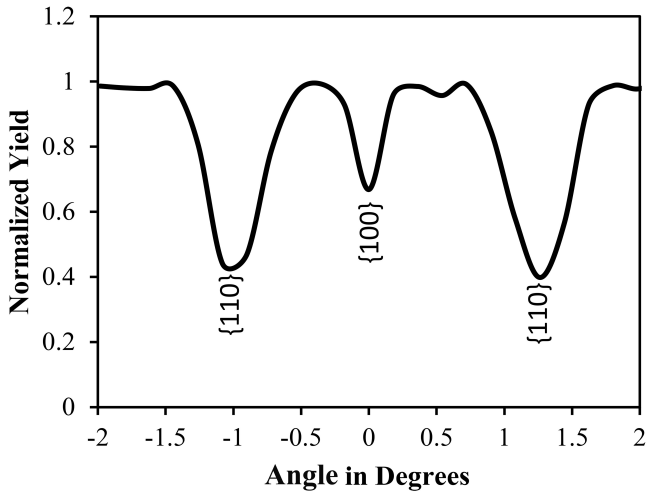

Figure 1: The normalized yield as a function of the angular scan of Si $< 100 >$.

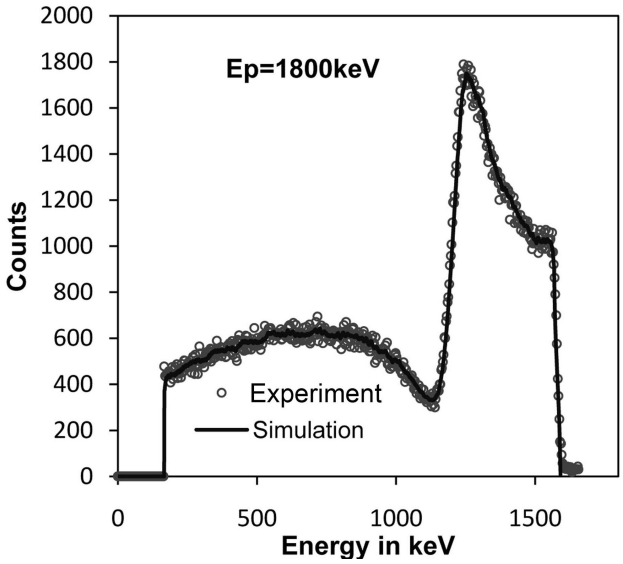

Figure 2: Experimental and simulation spectra of protons in the random direction of Si.

2 Materials and Methods

2.1 *Experimental procedure*

The Si crystal wafer cut in the direction of the plane (100) was cleaned and etched 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 of less than 0.06°. The Si surface barrier detector was employed at the angle $\theta = 165°$ with respect to the incident beam. The nominal energy resolution of the detector was 15 keV. The proton ion beam with different energies was produced by a 3 MV Van de Graaff accelerator. The {100} and the {110} planar directions were determined by an angular scan of the target. The normalized yield as a function of the angular scan of the target is shown in Fig. 1. The spectrum of each direction was taken in the energy interval 1400 to 2200 keV at the tilt angle at which the backscattering particle count was the minimum. Random spectra were taken 3° away from the planar directions.

2.2 *Theory*

The method used for simulating the channeling backscattering Rutherford spectra has been described in detail by Aslanoglou et al. (Aslanoglou et al., 1998). The foundation of the simulation procedure has been established on the assumption that dechanneled particles follow the exponential pattern:

$$N_d = N_0\left(1 - \exp(-\frac{x}{\lambda})\right) \quad (1)$$

where N_0 is the initial number of ions in the channel and λ is the mean channeling distance, which is considered an

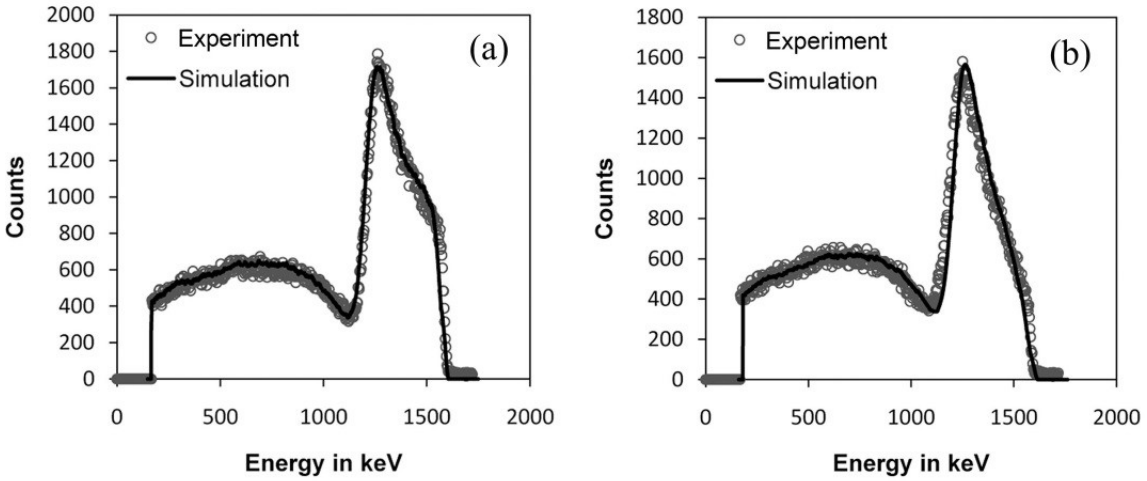

Figure 3: Experimental and simulation of channeling spectra along the a) {100}, and b) {110} directions.

energy-independent parameter. The number of ions escaping from the channel at a depth between x and $x + \mathrm{d}x$ is expressed by the following:

$$\mathrm{d}N_d = \frac{N_0}{\lambda}\, \mathrm{e}^{-\frac{x}{\lambda}}\, \mathrm{d}x \tag{2}$$

The dechanneling rate is a constant parameter given by (Kokkoris et al., 2003):

$$k \equiv \frac{1}{\lambda} \tag{3}$$

The simulation program was written in the standard language C++. For the calculations, the target was divided into slices of thickness $\mathrm{d}x = 0.02$ μm. In each slice, the number of dechanneled particles and their energies were evaluated. It was noted that the channeled particles suffer only a portion of the energy loss of the random part.

$$\left(\frac{\mathrm{d}E}{\mathrm{d}x}\right)_{Channel} = \alpha \left(\frac{\mathrm{d}E}{\mathrm{d}x}\right)_{Random} \; ; \; 0 < \alpha < 1 \tag{4}$$

The dechanneled beam was considered a random component, and its stopping power was calculated using the Ziegler formula and approximation (Ziegler et al., 2010).

The energy of ions when left the target regarding the backscattering in each former slice was calculated using the following:

$$\begin{aligned} E_{out} = & k\Big[E_0 - \Big(\int_0^{x_{ch}} \alpha\left(\frac{\mathrm{d}E}{\mathrm{d}x}\right)\mathrm{d}x + \int_0^{x_R}\left(\frac{\mathrm{d}E}{\mathrm{d}x}\right)\mathrm{d}x\Big)\Big] \\ & - \int_0^{x_{ch}+x_R/\cos\theta}\left(\frac{\mathrm{d}E}{\mathrm{d}x}\right)\mathrm{d}x \end{aligned} \tag{5}$$

where x_R and x_{ch} are the distance, ions pass in the random direction and through the channel before being dechanneled, respectively. The number of backscattered ions is given by the following:

$$N_{\mathrm{det}} = N_{\mathrm{inc}} \times \left(\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right) \times N_{\mathrm{target}} \times \Delta\Omega \tag{6}$$

$$N_{\mathrm{target}} = \left(\frac{A_\nu \rho}{A}\right)\left(\frac{\mathrm{d}x}{\mathrm{d}E}\right)\mathrm{d}E \tag{7}$$

where N_{inc} is the number of incident ions, A_ν and A are Avogadro's number and mass number of ions, respectively, and ρ is the target density. It noted that for the channel part of the beam, the value of $\mathrm{d}N_d$ should be considered in Eq. (6).

To take the multiple scattering and the beam straggling into account, the energy dependence of the elastic cross-section of the reaction ^{28}Si(p,p)^{28}Si was obtained from the excitation function, extracted from the random experimental spectra (Aslanoglou et al., 1998). The random spectrum counts contain differential cross-section times the target thickness $\mathrm{d}x$, the number of atoms in the target, and the experimental setup data information such as the number of incident particles and the solid angle of the detector. The spectrum counts were transferred to the elastic cross-section via the experimental setup data and the above-mentioned parameters. Since the calculation of the experimental setup data leads to an error in determining the simulation parameters, the random spectrum counts, which carry the setup information, were directly used as the number of backscattered ions. Figure 2 shows that this excitation function can reproduce the random spectrum precisely.

The energy resolution of the detector was also included in this program. The simulation was done in the energy interval 1400 to 2200 keV. In each energy, a set of parameters, α and λ, in which the least-squares achieved was picked as the best using the Levenberg-Marquardt method (Madsen et al., 2004). Then, the average value of channeling parameters concerning their errors in this energy interval was taken as the intended parameters in each crystallographic direction.

3 Results and discussion

The experimental channeling spectrum of protons at the energy of 1800 keV, for instance, along the {100} and the {110} crystallographic directions with simulations is shown in Fig. 3. The simulated spectra demonstrate great consistency with the experimental results.

Table 1: Values of α and λ along the {100} and the {110} planar directions of Si.

	Lattice direction	E (keV)					Average	Other works
		1400	1600	1800	2000	2200		
α	{100}	0.92 ± 0.01	0.9 ± 0.02	0.93 ± 0.02	0.9 ± 0.02	0.92 ± 0.02	0.92 ± 0.01	0.88 ± 0.04
	{110}	0.82 ± 0.02	0.8 ± 0.02	0.81 ± 0.03	0.79 ± 0.01	0.81 ± 0.01	0.8 ± 0.01	0.82 ± 0.04
λ (μm)	{100}	0.44 ± 0.11	0.42 ± 0.05	0.49 ± 0.06	0.43 ± 0.02	0.47 ± 0.1	0.440.02	-
	{110}	1.72 ± 0.05	1.64 ± 0.06	2.23 ± 0.04	2.26 ± 0.13	2.52 ± 0.07	2.030.02	-

The values of α and λ along the {100} and the {110} crystallographic directions of Si in the energy interval 1400 to 2200 keV are illustrated in Table 1.

By considering the uncertainty, the calculated average values of in this paper along the planar channels of Si are all in remarkable agreement with the values obtained in the literature. This confirms the validity of our simulation and subsequently the validity of the calculated values of λ. Taking into account the average value of λ along the {100} and the {110} channels, it is possible to calculate the dechanneling rate, k. The dechanneling rate in the {100} and the {110} directions is calculated at about 2.27 μm^{-1} and 0.49 μm^{-1}, respectively.

Figure 4 indicates the proportion of the experimental RBS and RBS/C spectra of the proton ions at the energy of 1800 keV in the Si. It shows that the back-scattering yield along the {100} plane decreases slightly near the surface of the target. It means that the dechanneling ratio of protons along this channel falls sharply and most ions escape the channels after traveling a very short distance through the channel. Then, the dechanneled ions follow the histories of the random ions in the target. Subsequently, the channel spectrum approaches the random one. As a result, the mean distance that ions travel along the channel is low. In addition, the difference in the energy at which the resonance peaks appear at random and the {100} spectra, is not clear. So the energy loss of ions in the {100} channel is almost the same as the random one. As shown in Table 1, the calculated value of α is near the random stopping power.

The RBS/C spectrum of protons along the {110} direction illustrates that the dechanneling ratio of protons along the {110} channel follows a moderate decline and the back-scattered yield of ions along this channel decreases visibly around the energy in which the resonance peak is seen. Therefore, ions along the {110} channel travel longer distances than those travelling through the {110} channel. Moreover, the resonance peak in the {110} spectrum appears at lower energy in comparison with the random spectrum. So the ions along the {110} plane of Si have less channeling stopping power than the ones along the random ions. The values of α and λ in Table 1 also confirm that.

The difference in the dechanneling parameters along the planar channels shows the various ion-atom close-encounter collisions along the channels. The anomalous behavior of the channeled ions is due to the regular arrangement of atoms along the lattice of a crystal. This arrangement not only provides an open area for the ions travelling in the sample but also produces an atomic force confining the channeled ions in the region far from the atoms. Since the {100} channel has smaller interplanar spacing than the {110} channel, it had less open area in comparison with the {110} channel. The ions travelling through the {100} channel experience the most interactions with the atoms. As a result, ions lose more energy by penetrating into the {100} crystal's direction in comparison with those penetrating into the {110} channel. Furthermore, ions along the {100} channel get enough energy to overcome the atomic force in the channel and escape the channel by travelling a very short distance along the channel.

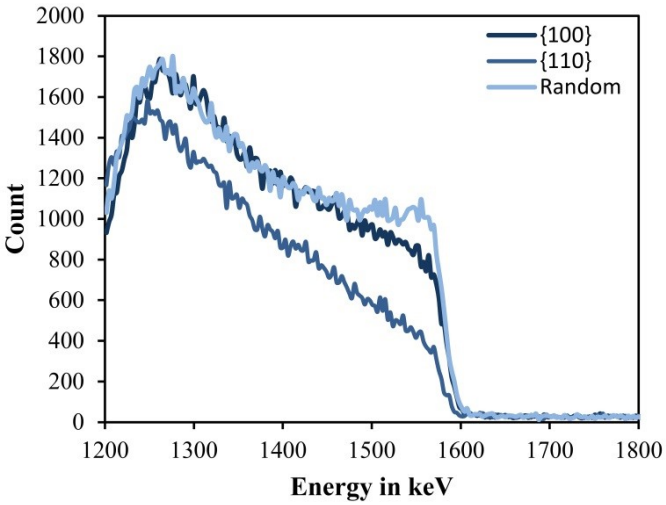

Figure 4: The experimental channel and random RBS spectra of the proton ions at the energy of 1800 keV in Si.

4 Conclusions

In this study, the characteristic behavior of the protons in the energy range of 1400 to 2200 keV along the {100} and the {110} planes of Si have been investigated by simulating the measured RBS/C spectra. The simple exponential dechanneling function reproduces the RBS/C spectra very well. The ion solid interactions along the channel are described by the means of two parameters: the ratio of channeling to random stopping power, α, and the mean channeling distance, λ. The parameters are independent in the energy interval of 1400 to 2200 keV. The values of α are in good agreement with those reported in the literature for lower energies. The mean channeling distance along the planar directions of Si is noticeably less than the corresponding axial channel calculated by Aslanoglou

et al. (Aslanoglou et al., 2000). This shows the difference between the nature of the ion-solid interactions along the axial and the planar channels. Comparison of the {100} channel with the {110} channel shows that the longer interplanar spacing of the {110} channel causes the larger atomic force on the ions along this channel. Therefore, ions along the {110} channel are confined tightly in the center of the channel and experience lower interactions with the electrons of the atoms. This leads to a lower energy loss and a longer mean channeling distance in the {110} channel than the ones in the {100} channel.

Conflict of Interest

The authors declare no potential conflict of interest regarding the publication of this work.

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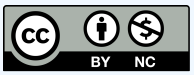

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