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Simulations and Comparisons of Channeling Spectra in the $p+^{28}\text{Si}$ System in the Backscattering Geometry

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Abstract

A new method has recently been proposed for the simulation and analysis of channeling spectra in the backscattering geometry [1], based on reaction cross sections and the assumption that beam particles escape from the aligned direction at an exponential rate. The success of the method in the system $p+^{28}\text{Si}$ cut along the $\langle 100 \rangle$ plane [2] led to the investigation of more complicated crystal structures and beam-target combinations, namely $\alpha+\text{MgO}$ and $\alpha+\text{Al}_2\text{O}_3$, which revealed the prospects as well as the limitations of the method [3].

In the present work channeling spectra of protons in a ^{28}Si crystal cut along the $\langle 111 \rangle$ plane, in the energy region $E_p = 1.7\text{-}2.4$ MeV are studied and analyzed. The measured backscattering spectra are reproduced by computer simulations and an attempt is made to describe the differences between the $\langle 100 \rangle$ and the $\langle 111 \rangle$ axis in the silicon crystal and their subsequent effect on the stopping power of channeled protons. The results are compared with those of methods reported in the past at different energy regions of the incoming protons [4,5].

1 Introduction

In the early 1960's, it had been observed [6,7] that the energy loss of positively charged particles incident on crystalline materials at an angle close to a low

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index axis or plane consists of only a fraction of the energy loss in a random direction of incidence. This was explained by Lindhard [8] with the low charge density in the channel, leading to a lower energy loss. According to this theory, a value of 0.5 is expected for ϵ , the ratio of the energy loss for channeled versus randomly incident particles. Values for this ratio, reported for many crystals in a variety of experiments, range from 0.3 to 0.7. For thick crystals Backscattering Geometry must be used and a resonance of the reaction proves to be a good marker for the range [9]. With this technique a value around $\epsilon = 0.65$ for Si has been recently reported [4]. Interpretation of the data, however, required lengthy Monte-Carlo calculations.

A new effort has recently been undertaken to describe the process using only two parameters, namely ϵ , the ratio of stopping powers in the channeling and random directions and λ , the mean channeling distance. The initial success of a "linear approximation" applied to a silicon crystal [2], led to further development of the analysis tools and their application to crystals of Si $\langle 100 \rangle$, MgO and Al₂O₃ [3].

The results presented here concern another silicon crystal cut in the $\langle 111 \rangle$ direction. The aim of this work is to test the validity of the method and to compare the behavior of two different crystal channels in silicon, as far as the stopping power of incident protons and their corresponding mean channeling distance are concerned.

2 Data Analysis

A program was written [2], which divides the target into slices and splits the beam into a channeled and a dechanneled component. It then follows the evolution of the two components through the target. At each slice the channeled component enters with energy E_c and it loses energy at the rate of $\epsilon \cdot S(E_c)_{\text{rnd}}$ where ϵ is assumed energy independent and $S(E_c)_{\text{rnd}}$ is the specific energy loss calculated with the coefficients of Ziegler [10] in the amorphous material. This component also loses flux at a constant rate, which is equivalent to an exponential decay of the channeled flux.

The dechanneled component enters the slice with energy E_d and loses energy at the rate of $S(E_d)_{\text{rnd}}$. Its flux increases by the amount of beam dechanneled in the previous slice. If a constant dechanneling rate λ is assumed it leads for the flux N_d to:

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

where λ is also considered energy independent. The elastic scattering cross

section [2] is used to compute the amount of beam scattered to the detector direction. This component is then transported through the crystal assuming random specific energy loss and a simulated channeled spectrum is generated and compared to the experimental data. The program is written in standard FORTRAN and runs on any computer. The simulated spectrum is written to file and can be displayed by a general purpose graphic interface. Provision is also made, for the incorporation of the program within the frame of the MINUIT minimization package, which allows automatic search for the values of ϵ and λ giving the best fit.

3 The Problem of the Excitation Function

The number of backscattered particles by a portion of the target of thickness dx at depth x is governed by the reaction cross section at that energy which can be considered to be the same as in the random case. In this work, our goal was to use elastic scattering cross sections together with the dechanneling mechanism described above to reproduce the experimental spectra. The cross sections used had to reproduce the experimental spectra in an accurate way at the random mode, in order to eliminate any ambiguity regarding the cross section. Thus, the only difference between the spectra in the aligned and random mode was the dechanneling process. Excitation function data for the elastic scattering $p+^{28}\text{Si}$ can be found in the literature, or can be extracted from the random orientation spectra. In the present case, no data exist for the reaction $p+^{28}\text{Si}$ at $\Theta = 160^\circ$ (detector angle), the nearest case of excitation function data being those presented by Vorona et. al [11], at $\Theta = 170^\circ$, which can not be taken as a priori accurate for $\Theta = 160^\circ$. In a trial calculation it was observed that the random orientation spectra at $\Theta = 160^\circ$ are well reproduced by these excitation functions for the case of the $E_p = 1.67$ MeV resonance, but not for the one at $E_p = 2.09$ MeV. Evidently, this happens because the resonance at 2.09 MeV is much narrower than that at 1.67 MeV, and small deviations in the cross section due to the 10° difference produce greater differences in the simulations.

Excitation functions were thus constructed from the random orientation data, and were subsequently used as input for the channeling case (the spectra always taken at the same E_p), with the use of a computer code. The cross section deduced this way from the deconvolution of the experimental spectra, included distortions originating from effects connected to the thick target yield, such as energy straggling of the beam and multiple scattering. These effects however, were the same for either the random or channeling mode, so the validity of the method is preserved.

The basic philosophy followed, is the same as in the simulation of the random

spectra. For each block of the target of thickness dx at depth x , the beam energy of entrance and exit of the block $E_{x,in}$ and $E_{x+dx,in}$ were calculated. Then, the corresponding detected particle energies $E_{x,out}$ and $E_{x+dx,out}$ were computed, in a way similar to that of the simulation of the spectra. In this way, a relation was established between the energies E_{out} of the experimental spectrum and the interaction energy E_{in} . The number of events in the experimental spectrum in the energy bin between $E_{x,out}$ and $E_{x+dx,out}$ was then transformed to cross section data and registered at energy E_x . The transformation from spectrum counts to cross section was done via the experimental set up data (detector solid angle, target thickness dx , integrated charge etc).

4 Experimental Results

The experiments were performed at the N.C.S.R "Demokritos", Athens, Greece, using the TN11 TANDEM Accelerator. The scattering chamber used included a goniometer system (RBS-400 by Charles Evans Co) capable of determining the target orientation with an accuracy of 0.01° . The detection system consisted of a single Si surface barrier detector placed at an angle $\Theta = 160^\circ$ with respect to the beam, holding an overall resolution of 18 keV. The target used was a Si crystal wafer, cut at the direction of the plane $\langle 111 \rangle$. Before the measurements, a polar and an angle scan were performed in order to align the beam to the $\langle 111 \rangle$ string of the crystal. The channeling angle was found to be approximately 0.4° . For the polar scan, the target was tilted by 3° and rotated around the beam axis. The results are presented in Figs. 1 and 2.

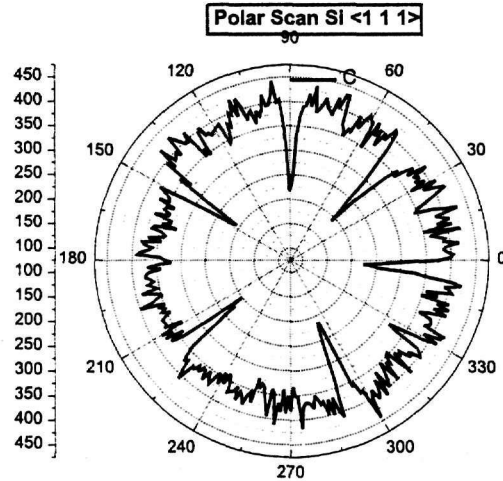


Fig. 1. Polar scan of the Si $\langle 111 \rangle$ crystal

Spectra of protons back scattered at angle $\Theta_{lab} = 160^\circ$ were taken at the energy

interval $E_{lab} = 1.7 - 2.4$ MeV in steps of 50 keV, in both random and aligned angles of incidence. The reaction $^{28}\text{Si}(p,p)^{28}\text{Si}$ exhibits two sharp resonances in that energy interval at energies $E_{lab} = 1.67$ MeV and 2.09 MeV, having natural widths $\Gamma = 52.0 \pm 0.8$ and 15.6 ± 0.6 keV respectively [11]. Experimental spectra along with the simulations in the aligned mode at energies $E_{lab} = 2.40$, 2.20 and 1.75 MeV are presented in Figs. 3, 4 and 5. The 1.67 MeV resonance appears clearly in the spectrum at $E_p = 1.75$ MeV. At $E_p = 2.20$ MeV, the 1.67 MeV resonance is smeared out, while the 2.09 MeV one appears sharp. At $E_p = 2.40$ MeV, only the 2.09 MeV resonance remains visible. The reproduction of the experimental spectra is quite satisfactory in all cases. The final results for ϵ and λ are presented in Figs. 6 and 7.

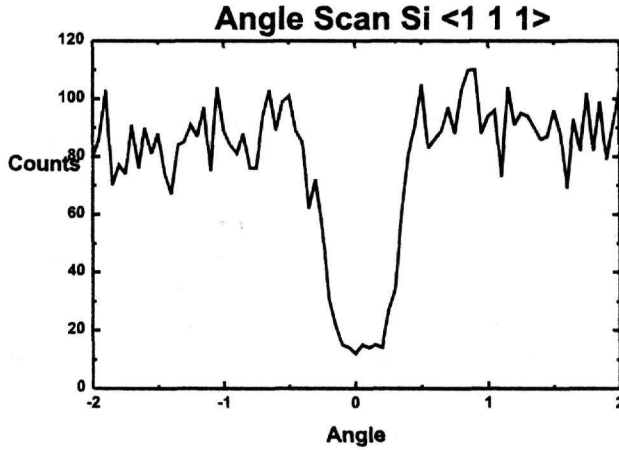


Fig. 2. Angle scan of the Si $\langle 111 \rangle$ crystal

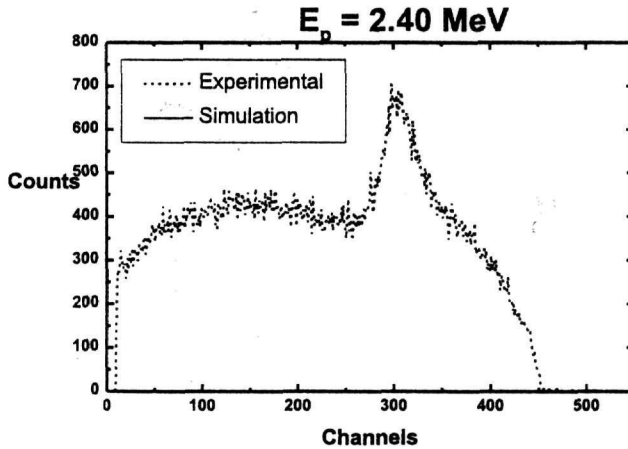


Fig. 3. Experimental and Simulation spectra at $E_p = 2.4$ MeV

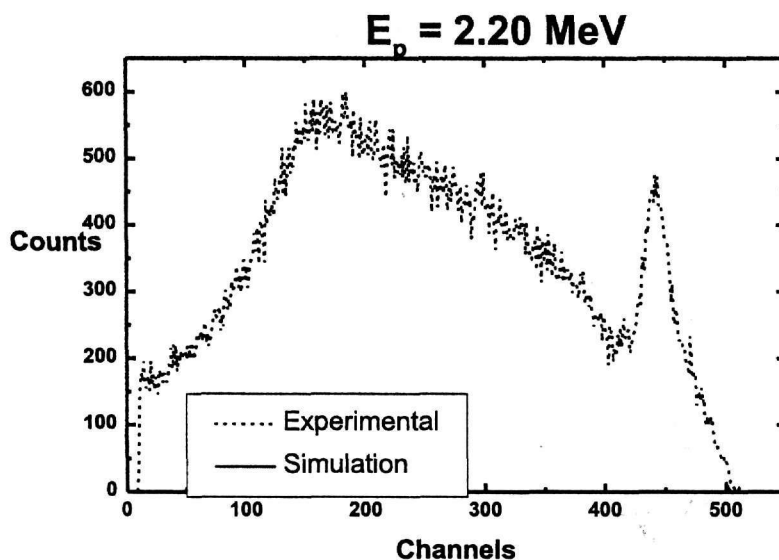


Fig. 4. Experimental and Simulation spectra at $E_p = 2.2 \text{ MeV}$

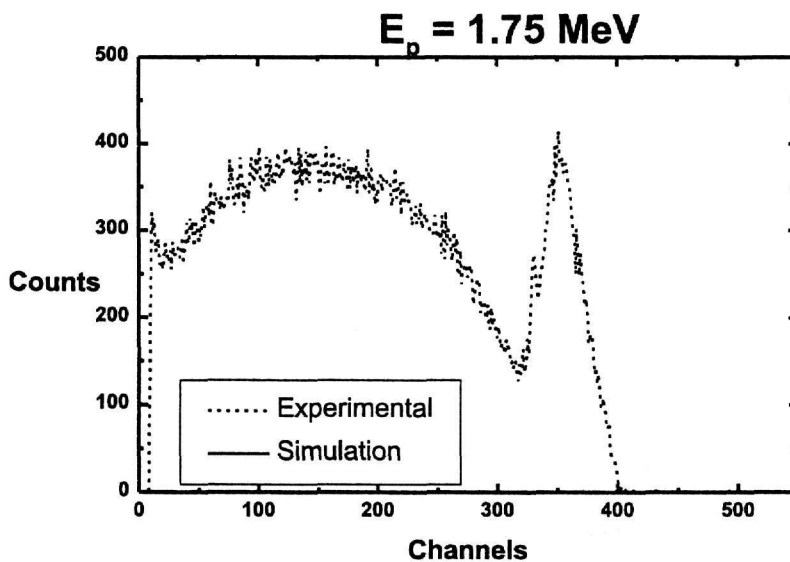


Fig. 5. Experimental and Simulation spectra at $E_p = 1.7 \text{ MeV}$

Si <1 1 1>

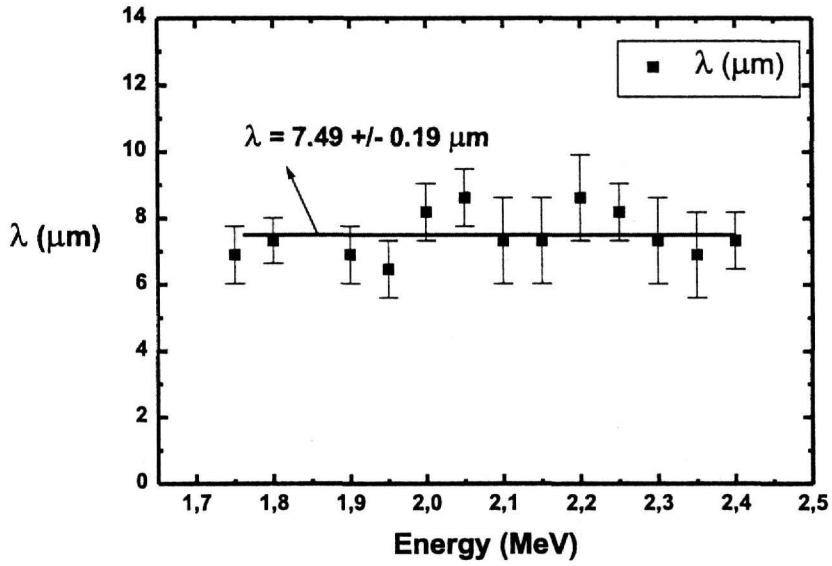


Fig. 6. λ (in μm) as a function of E_p (in MeV)

Si <1 1 1>

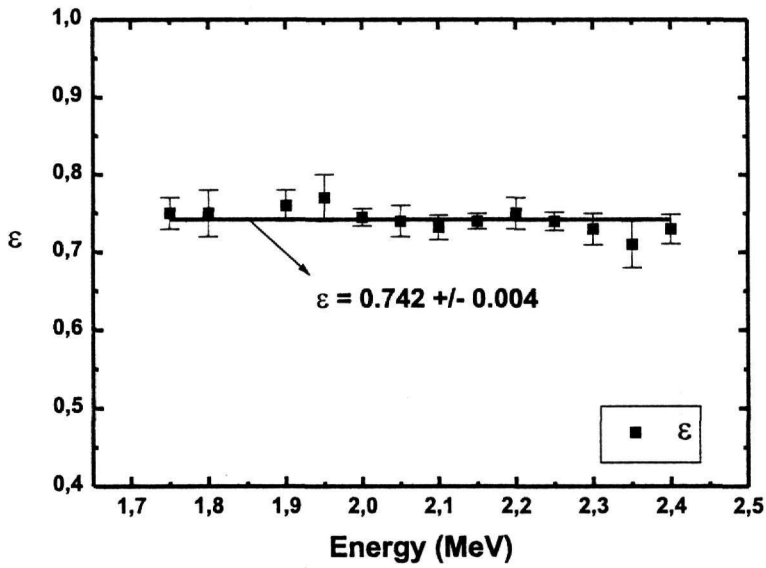


Fig. 7. ϵ as a function of E_p (in MeV)

5 Discussion and conclusions

The method presented here, is based on the assumption that dechanneling of beam protons follows an exponential law, which is characterized by the mean channeling distance. The rate of energy loss of particles moving along a low index axis of the crystal is only a fraction of that of the random direction. The accuracy of the parameters deduced from the simulations depends critically on the accuracy of the cross sections used. If accurate cross sections are not available, one measurement in random orientation can provide the thick target cross section needed.

Unlike methods reported in the past which rely on the presence of a resonance in the spectrum, in the present method the existence of a resonance in the system is not a requirement. However, the reproduction of an anomaly in the spectrum, such as a resonance, increases the accuracy of the method.

The data analyzed in the energy range $E_p = 1.7\text{-}2.4$ MeV do not show any particular trend with regard to energy dependence of the parameters. The values of the parameters in this energy interval produce an average of $\lambda = 7.49 \pm 0.19$ μm and $\epsilon = 0.742 \pm 0.004$ for the $\langle 111 \rangle$ silicon axis. There are clear differences between these values and the ones calculated for the $\langle 100 \rangle$ silicon axis [2], namely, $\lambda = 9.54 \pm 0.24$ μm and $\epsilon = 0.691 \pm 0.003$.

Although these two parameters, λ and ϵ , are in a way related, we can make the assumption that ϵ is rather connected to the nature of the crystal channeling axis, while λ offers a measure of the quality of the general crystal structure. In that aspect, comparing the two crystallographic directions we could conclude that the stopping powers of channeled protons are similar, with the $\langle 100 \rangle$ axis producing a slightly stronger channeling effect. On the other hand, comparing the λ values, it is obvious that the $\langle 111 \rangle$ silicon target's crystal structure is clearly distorted. This corroborates with the fact that the target was part of a used surface barrier detector; thus, a significant number of dislocations of the atoms is expected to affect the channeling procedure. The $\langle 100 \rangle$ target [2] was a virgin crystal and the fact that the method used is capable of showing these differences, in an indirect manner, is quite impressive.

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