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THE RELATION BETWEEN DEPTH AND ENERGY IN CHANNELING EXPERIMENTS

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Spectra of protons backscattered from a silicon single crystal were measured at a bombarding energy of 2300 keV. A narrow resonance in the elastic scattering cross sections of protons from ^{28}Si, at 2090 keV, shows up as a peak in the spectra. The position and the shape of this peak were found to vary when the beam alignment was changed from a random to an axial or planar crystal direction. These effects are attributed to a different energy loss distribution of the incoming protons in these three cases. The measured spectra were compared with spectra obtained from Monte Carlo simulations in which the dependence of the energy loss on the impact parameter of the collision is taken into account. The measured and simulated spectra were found to agree qualitatively. By analysing the energy loss of the simulated trajectories, conclusions are drawn about the influence of the reduced energy loss in channeling directions on the energy to depth conversion in channeling experiments.

1. Introduction

The RBS/channeling technique is often used for defect depth profiling. In these experiments one usually assumes that the random and channeled stopping powers are equal. However, it has been known for a long time that the energy loss of channeled particles differs from the random (amorphous) case (see e.g. refs. [1–5]). Usually the defect depth distribution is broad and the assumption of equal stopping power for channeled and random particles does not lead to inconsistencies. If the defects are positioned at a well defined depth, deviations have been observed between the measured and expected defect depth [6,7], that may be attributed to the reduction of the stopping power in the channeling direction. The influence of the stopping power of channeled particles on the depth scale in an RBS/channeling experiment is discussed by several authors [8–10].

If one combines existing theories on the dependence on the impact parameter of the energy loss with a Monte Carlo program calculating the trajectories of channeled particles it is possible to compare measured and calculated energy loss distributions. In the experiments described in this paper a resonance in the cross section for scattering of protons from Si is used to study the energy loss of channeled particles. Measured channeling spectra are compared with computer simulations. Finally, the implications of the reduced energy loss on the damage profiles obtained by the RBS/channeling method are discussed.

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2. The energy loss of channeled particles

The stopping power of channeled particles differs markedly from that of particles following random trajectories. For protons with energies in the order of 1 MeV the stopping power is practically determined by electronic stopping only, and decreases slowly with increasing particle energy. If the beam is directed along a major string or plane, most ions will follow channeled trajectories and the particle flux will be largest in the center of the channel. The low electron density in the center of the channel will cause a reduction of the stopping power. For the best channeled particles the stopping is reduced to 25–50% of the random value. Particles with a higher transverse momentum follow oscillating trajectories and will probe also the areas with higher electron densities. The stopping of these particles will be close to the random value. Besides the average energy loss also the second moment of the energy loss distribution (the straggling) is of importance. It will influence the depth resolution of the damage depth profiles. In an amorphous solid the straggling is described approximately by the Bohr theory [10]. According to this theory the spread in energy loss is a Gaussian with a width increasing with the square root of depth. In a single crystal when the incident beam is aligned with a channel the energy loss is different for the different kinds of trajectories and the width of the energy loss distribution increases roughly linearly with depth.

If one uses channeling for depth profiling of defects the consequences of the deviating energy loss of channeled particles for the depth scale and the depth resolution should be considered carefully. One may divide the trajectories of the ions at a depth z into four classes:
(1) trajectories dechanneled at the surface;
(2) trajectories initially channeled but dechanneled before reaching depth z;
(3) trajectories poorly channeled at depth z;
(4) trajectories well channeled at depth z.

Particles of classes 1 and 2 have a random probability of backscattering at depth z and do not provide information about the defects at depth z. Consequently their energy loss is of no importance for the determination of the depth z of the defects.

Particles of the poorly channeled fraction at depth z (class 3) have an energy loss varying from about equal to the random case (if the particle was channeled poorly right from the beginning) to almost equal to the well channeled case (if it became poorly channeled just before reaching depth z). These particles have a high probability of dechanneling, because they need to gain only a small amount of transverse momentum.

Well channeled particles have the lowest energy loss. They will not easily dechannel by strain-like defects but they do contribute to the yield from displaced atoms.

Thus depth profiles of strain-like defects are related to the energy loss of trajectories of class 3 and only for a minor part also to the trajectories of class 4. The depth profiles of defects causing direct scattering will be influenced by both the energy losses of class 3 as well as class 4.

3. The spectra of protons backscattered from a Si crystal

A simple experiment was done in which the energy loss distribution of protons in a perfect Si crystal is probed for various incident directions. The cross section for elastic scattering of protons from a ^{28}Si nucleus shows a strong resonance at $E_p = 2090$ keV [12]. First, this differential cross section at a fixed angle was measured for a thin target. A thin layer (22 μg/cm^2, corresponding to an energy loss for 2 MeV protons of 2.3 keV) of silicon with the natural isotope composition was evaporated onto a carbon backing. Due to the difference in kinematic factor protons backscattered from Si are well separated in energy from protons backscattered from C. Except for oxygen, no impurities were detected in significant amounts. Fig. 1 shows the scattering yield from Si as a function of bombarding energy for a detector placed at a laboratory angle of 165°. At an energy of 2090 keV a large peak (with a width of approximately 18 keV) is observed, preceded by a minimum. This anomaly in the scattering cross section is caused by the excitation of, and elastic re-

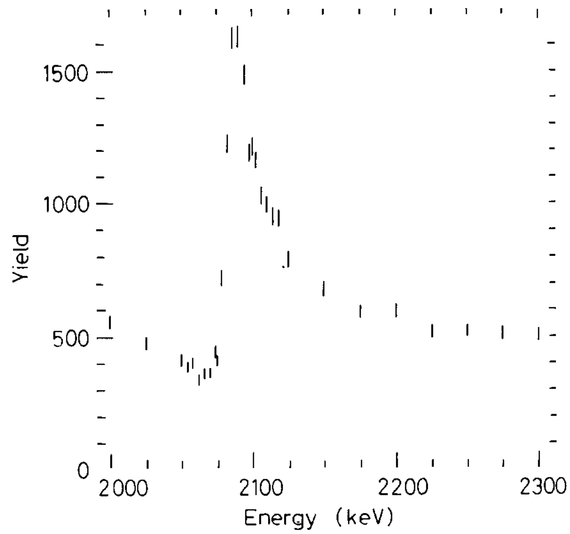

Fig. 1. The thin target yield of protons backscattered from Si as a function of bombarding energy. The scattering angle was 165°.

emission from an excited state of the ^{29}P nucleus. This process interferes destructively (for $E_p < 2080$ keV) or constructively (for $E_p > 2080$ keV) with the Rutherford scattering. These measurements agree with the data of Vorona et al. [12].

Subsequently the target was replaced by a Si crystal with a ⟨100⟩ surface normal. Backscatter spectra were taken with exactly the same scattering angles with the beam aligned with the ⟨110⟩ string, the (111) plane, and a random direction. The (111) planar and random spectra were taken 3° away from the ⟨110⟩ string. For the energy of the incoming particles a value of 2300 keV was chosen. When the proton energy has decreased by the electronic stopping to a value of 2090 keV, the backscatter probability increases. This causes a peak in the spectra of the backscattered protons. The energy of the peak in the backscatter spectrum is given by:

$$E_f = K^2 E_r - \int_0^l S(E')\, \mathrm{d}r = K^2 E_r - \Delta E_{out} \quad (1)$$

with $E_r = 2090$ keV, K^2 the kinematic factor, $l = z/\cos\beta$ where β is the angle between the outgoing trajectory and the surface normal. $S(E')$ is the random stopping power. Thus, by measuring the energy corresponding to the peak in the backscatter yield, the mean depth z at which the energy of the incoming particles is reduced to 2090 keV is determined. In fig. 2 the spectra of the backscattered particles are shown for the incident beam aligned with a random, the (111) planar and the ⟨110⟩ axial direction. It is clear that the peak position for the axial case differs from the other cases. Thus the effective stopping power is lower in the ⟨110⟩ axial direction. The effective stopping in the (111) planar direction is hardly different from the random case. The

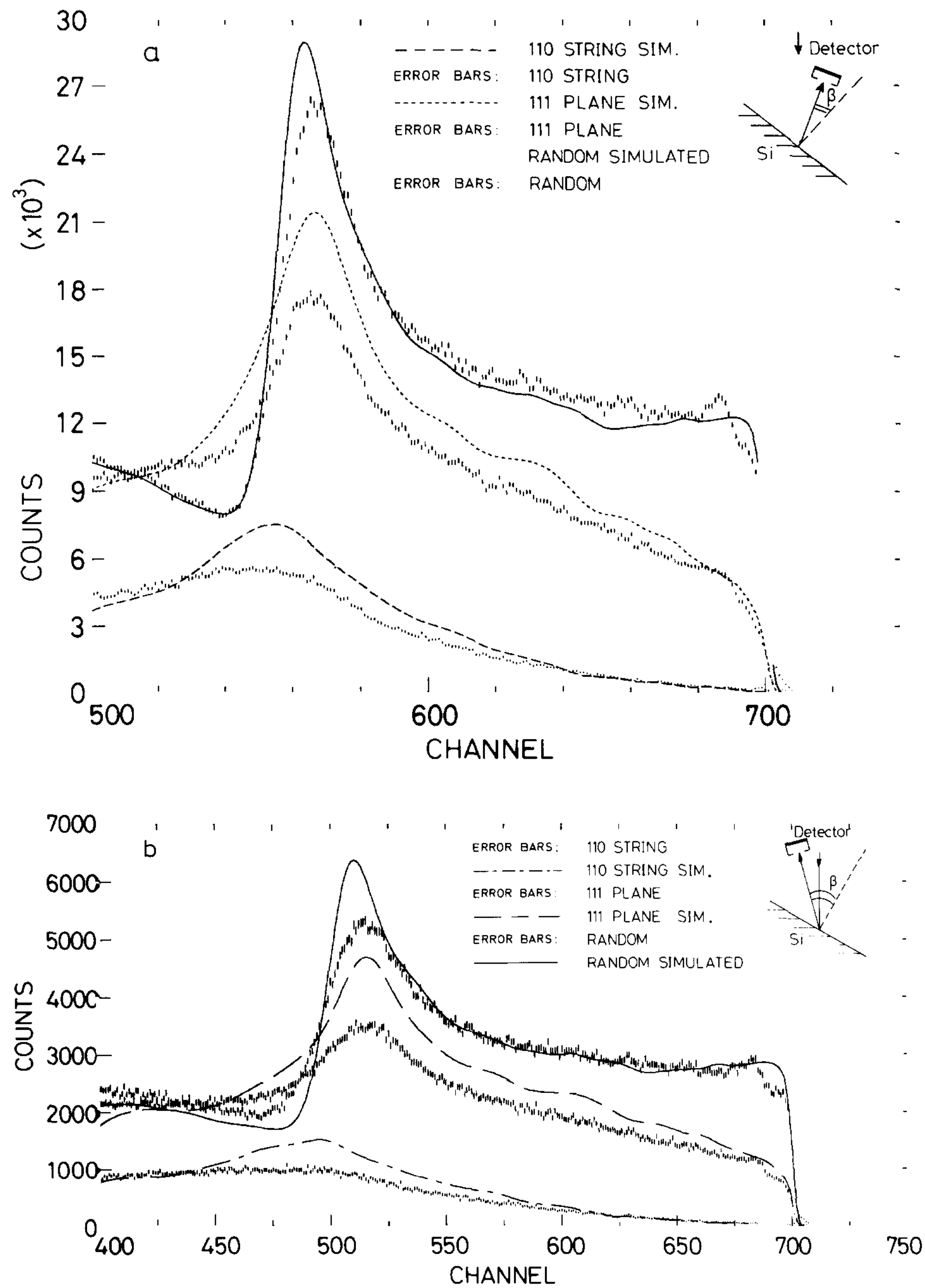

Fig. 2. Measured and simulated spectra of 2.3 MeV protons backscattered from a Si crystal. The random, (111) planar and ⟨110⟩ axial spectra are shown. For both (a) and (b) the scattering angle was 165° but the detector in case (b) was situated at a more glancing angle (geometry as indicated).

most striking difference is the shape of the peaks. In the random case the shape of the peak still resembles the shape of the thin target yield. In the planar and axial case the broadening is much larger. Also a tail at the low energy side is clearly observed, obscuring the minimum that preceded the peak in the random spectrum. It is caused by particles with a lower energy loss on their incoming trajectories. The backscatter probability of well channeled particles is strongly reduced. Thus mainly particles that are dechanneled when reaching the resonance energy (class 1 and 2) will contribute to the peak in the spectrum.

4. Simulations

In a Monte Carlo calculation different trajectories have different energy losses if one includes impact parameter dependent energy losses. This is done in a computer program developed by Smulders and Boerma [13]. In this program the trajectories of particles in single crystals are calculated. The deflection by the nearest atom is treated as a binary collision in the impulse approximation. The influence of the more distant strings of atoms is taken into account in the continuum string approximation. The electronic energy loss is divided into contributions from the inner shell electrons and from the valence electrons. The energy loss due to the the inner shell electrons depends on the impact parameter of the collision and is calculated as described by Dettmann and Robinson [14]. The valence electrons are assumed to be distributed uniformly over the channel. The energy loss to the valence electrons is caused both by distant plasma excitations and close scattering events and is implemented as described by Melvin and Tombrello [15].

To simulate the channeling spectra, the Monte Carlo program was modified in order to include the energy dependent cross section for backscattering. Besides the backscatter probability as a function of depth also the first and second moment of the energy distribution of the protons, weighted by the backscatter probability, were calculated. From this output an energy spectrum was generated, taking into account random stopping and straggling for the outgoing trajectories and the detector resolution (approximately 10 keV). To limit the complexity of the calculations the energy distribution of the incoming particles at the time of scattering is represented by a Gaussian at each depth.

The simulations were done for 2.3 MeV protons. The calculations took several days and were done as a background job on a Perkin-Elmer 3220 minicomputer. It turned out that the dechanneling rate was somewhat overestimated in the simulations. Thus the gain of transverse momentum due to the lattice vibrations and/or due to scattering by electrons is overestimated in the program. In order to get about the right dechanneling rate the rms vibrational amplitude was reduced from 0.075 to 0.068 nm. We believe that by this procedure some approximations applied in the model [13] such as the uniform distribution of valence electrons are compensated. From other simulation work we know that the inclusion of correlations in the thermal vibration amplitude would introduce only a small change in the dechanneling rate [13].

The simulated spectra are also shown in fig. 2. The simulated random spectra were normalised in such a way that the area of the measured and simulated random spectra are equal.

In order to get a better understanding of the energy loss of the channeled particles, the energy distribution of the ions at a depth of 8.5 μm was calculated. The

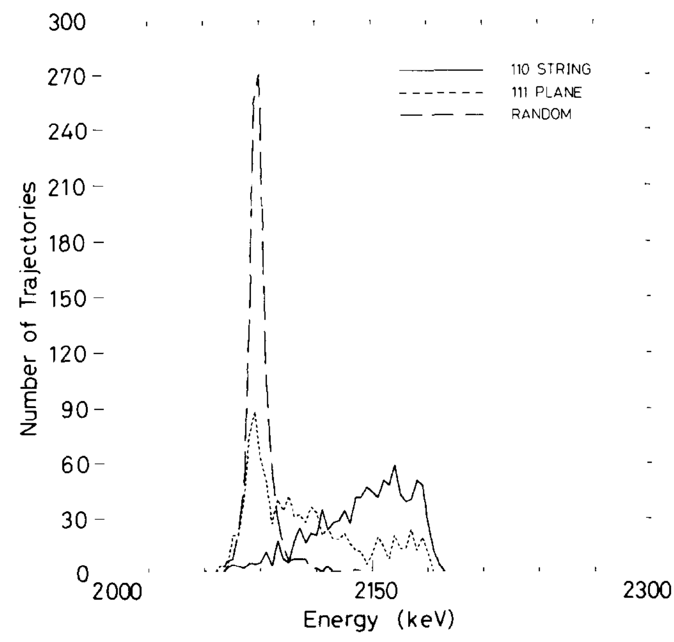

Fig. 3. The simulated energy distributions of 2.3 MeV after transmission through a 8.5 μm thick Si crystal with the ions directed along the ⟨110⟩ string, the (111) plane and a random direction.

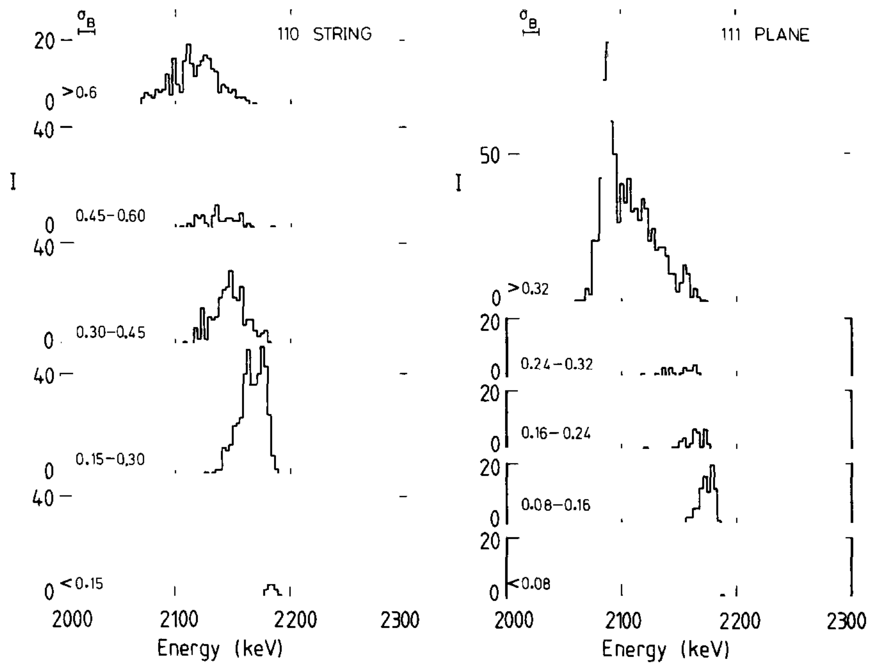

Fig. 4. The calculated energy distribution of protons transmitted through a 8.5 μm thick Si crystal for the ⟨110⟩ axial (left) and (111) planar (right) direction. The distribution is plotted for groups of trajectories with different maximum angles with the channeling direction as indicated. The critical angle for 2.3 MeV protons for the ⟨110⟩ string of Si is 0.39° and 0.11° or 0.19° for the alternating narrow and wide (111) planes respectively. The magnitude of the straggling as predicted by the Bohr theory (σ_b) is indicated as well.

energy of the nonchanneled particles is reduced to 2090 keV for this thickness. In fig. 3 the calculated energy distribution of particles at a depth of 8.5 μm is shown for the ⟨110⟩ string, (111) plane and a random case. The shapes of these calculated energy loss distributions compare well with the experimental energy loss distributions of protons transmitted in different directions through thin single crystals as measured by Appleton et al. [2]. In the simulations the stopping power of the best channeled particles is reduced to 55% of the random value both for the (111) planar and [110] axial channeling direction. From the measurements of Appleton et al. a reduction of the stopping power for the best channeled particles is estimated to be slightly more than 50% for protons in this energy range. The influence of channeling on the energy loss is clearly seen in this figure.

For the ⟨110⟩ string and (111) plane we divided the trajectories in different groups as a function of the largest angle between the trajectory and the channeling direction occurring during the first 8.5 μm of the trajectories. This is done in fig. 4. The best channeled particles experience the lowest energy loss as expected.

5. Discussion

A comparison of the measured and simulated random spectra shows that the resonance peak position is calculated correctly, but the area of the peak is overestimated in the simulations. Thus the calculated random stopping power seems quite correct. The random stopping power as calculated from fig. 3 is indeed equal to the literature value (25 eV/nm) [16]. The fact that the area of the peak is not predicted correctly, even in the random case, is somewhat surprising and not completely understood. It might be due to particles reaching the detector after more than one deflection [17]. Obviously the scattering cross section used is not valid for these trajectories.

The influence of channeling on the shape of the resonance is reproduced qualitatively by the simulations. In the simulated planar case the rate of dechanneling is somewhat too high. The broadening of the peak and the peak position are predicted correctly. In the stimulated spectrum for the axial case the broadening seems to be underestimated.

Although experiments and simulations do not agree quantitatively, the general features of the spectra are predicted correctly. Therefore we conclude that the calculated values of the channeled energy loss are rather good approximations of the actual values. Now we can estimate the influence of the reduced energy loss on damage depth profiles obtained with the RBS/channeling method.

The energy loss of the channeled trajectories can be estimated from fig. 4. As argued in section 2, for damage depth profiling at a depth z only the energy loss of the channeled fraction at depth z is of importance, i.e. only the lower 2 or 3 graphs of fig. 4 play a role. In this example the average energy loss of the channeled particles is reduced by 35% in both the axial and the planar case. The fact that the reduction of the average energy loss of the channeled particles is about 10% less than the reduction of the energy loss of the best channeled particles agrees with the conclusions of Eisen et al. [8] and Bøttiger et al. [10]. Due to the reduction of the incoming stopping power S_{in} by ΔS_{in} the depth z corresponding to a certain energy in the backscatter spectrum will be larger than the depth z', calculated using random stopping powers. The error may be estimated from

$$\frac{z'}{z} = 1 - \frac{\Delta S_{in}}{S_{in}} \left(1 + \frac{\cos \alpha}{K^2 \cos \beta} \frac{S_{out}}{S_{in}} \right)^{-1}. \quad (2)$$

Here S_{in} and S_{out} are the random stopping power averaged over the incoming and outgoing trajectories, the channeling stopping power is $S_{in} - \Delta S_{in}$, and α and β are the angles of the incoming beam and the outgoing particles with the normal of the surface. The expression between brackets is in the order of 1.5–5 in most practical situations. Thus the assumption of equal stopping for the channeled and random trajectories is likely to cause a underestimation of the defect depth by 5–20%, depending on the geometry of the measurement and the kinematic factor. Similar trends are found in the experimental results given in refs. [6] and [7]. From the width of the energy distribution of the channeled particles it is clear that the Bohr theory for straggling should not be used for channeling trajectories. Especially at large depth this would cause an overestimation of the depth resolution.

References

[1] G. Dearnaley, IEEE Trans. NS-11 (1964) 249.
[2] B.R. Appleton, C. Erginsoy and W.M. Gibson, Phys. Rev. 161 (1967) 330.
[3] G.G. Bentini, A. Carnera, G. Della Mea, A.V. Drigo, S. Lo Russo and P. Mazzoldi, Phys. Rev. B17 (1978) 3492.
[4] A.P. Pathak, Radiat. Eff. 61 (1982) 1.
[5] H.S. Jin and W.M. Gibson, Nucl. Instr. and Meth. B13 (1986) 76.
[6] M. Vos, D.O. Boerma, P.J.M. Smulders and S. Oosterhoff, Nucl. Instr. and Meth. B17 (1987) 234.
[7] G.G. Bentini, M. Bianconi and M. Servidori, Nucl. Instr. and Meth. B18 (1987) 145.
[8] F.H. Eisen, G.J. Clark, J. Bøttiger and J.M. Poate, Radiat. Eff. 13 (1972) 93.
[9] J.F. Ziegler, J. Appl. Phys. 43 (1972) 2973.
[10] J. Bøttiger and F.W. Eisen, Thin Solid Films 19 (1973) 293.
[11] N. Bohr, K. Dan. Vidensk. Selsk. Mat. Fys. Medd. 18 (1948) no. 8.
[12] J. Vorona, J.W. Olness, W. Haeberli and H.W. Lewis, Phys. Rev. 116 (1959) 1563.
[13] P.J.M. Smulders and D.O. Boerma, Nucl. Instr. and Meth. B29 (1987) 471.
[14] K. Dettmann and M.T. Robinson, Phys. Rev. B10 (1974) 1.
[15] J.D. Melvin and T.A. Tombrello, Radiat. Eff. 26 (1975) 113.
[16] H.H. Andersen and J.F. Ziegler, Stopping Powers and Ranges in all Elements, Vol. 3: Hydrogen (Pergamon, New York, 1977).
[17] J.A. Moore, Nucl. Instr. and Meth. 174 (1980) 577.