

## Fine Structure in Channeling Lines

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It is shown by calculations (classical treatment) that fine structure is to be expected in angular distributions of channeled particles. This fine structure will be superimposed on the normal smooth channeling line profile. It is due to coherent channeling. It requires high angular resolution and thin single crystals of uniform thickness for experimental detection. The fine structure pattern is sensitive to the details of the crystal potential.

### I. Introduction

The angular distribution of charged fast particles which have been channeled by the planes of a crystal is characterized by an intense narrow peak (channeling peak). This peak is superimposed on the much broader multiple scattering distribution originating from non-channeled particles.

Recent measurements<sup>1,2,3</sup> of the profile of such channeling lines (intensity distribution perpendicular to direction of the channeling plane) showed in each case a smooth curve with a shape similar to a gaussian distribution. These results are in accordance with theoretical considerations<sup>4</sup> which predict a smooth sinusoidal distribution, assuming a diffusion model. In this model the motion of the particles in the channels is governed by random walk processes.

The motion of channeled particles is, however, not only determined by such statistical diffusion processes, but is also subject to correlated deflections which result in well defined oscillatory particle paths between the crystal planes<sup>5</sup>. For such trajectories the phase of the oscillation at the exit surface of the crystal is correlated with the phase at the entrance into the crystal (coherent channeling). Therefore we expect deviations from the smooth angular distribution which is predicted by the diffusion model since it does not take into account the coherent particle oscillations. These deviations should show up most strongly in thin crystals since

the contribution from processes destroying the coherence is expected to still be moderate.

It will be shown in this paper on the basis of calculations (classical treatment) that coherent channeling will result in a fine structure with several maxima and minima in the angular distribution of the channeled particles. The details of this fine structure in channeling lines are sensitive to the potential between the crystal planes, i.e. the potential, which governs the motion of the channeled particles. Therefore the structure in the angular distribution may possibly be used to study crystal potentials.

The predicted fine structure maxima are normally very closely spaced. The angular resolution of the experimental arrangements used in the past does not seem to have been sufficient to resolve this structure. However high resolution experiments are expected to show the fine structure superimposed on the broader background of the normal (non-coherent) channeling distribution.

### 2. Calculations and Results

The fact that coherent channeling can lead to structure in the angular distribution can qualitatively be seen from very simple considerations. If we consider zig-zag beam paths (infinitely high square well potential), two maxima will result from such trajectories ( $\delta = \pm \alpha$ ,  $\alpha$  = incidence angle,  $\delta$  = emergence angle).

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<sup>1</sup> W. H. GIBSON, C. ERGINSOY, H. E. WEGNER, and B. R. APPLETON, Phys. Rev. Letters **15**, 357 [1965].

<sup>2</sup> B. R. APPLETON, C. ERGINSOY, and W. M. GIBSON, Phys. Rev. **161** (2), 330 [1967].

<sup>3</sup> B. R. APPLETON, L. C. FELDMAN, and W. L. BROWN, Proc. Intern. Conf. on Solid State Physics Research with Accelerators, Brookhaven Nat. Lab. 50083 (C-52) [1967].

<sup>4</sup> L. C. FELDMAN, B. R. APPLETON, and W. L. BROWN, Proc. Intern. Conf. on Solid State Physics Research with Accelerators, Brookhaven Nat. Lab. 50083 (C-52) [1967].

<sup>5</sup> H. O. LUTZ, S. DATZ, C. D. MOAK, and T. S. NOGGLE, Phys. Rev. Letters **17**, 285 [1966].



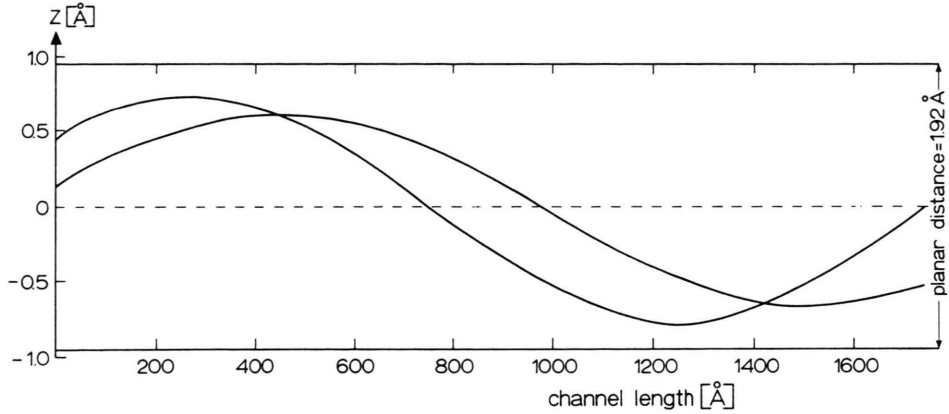


Fig. 1. Calculated paths of 3 MeV protons, coherently channeled between two (1, 1, 0)-planes of a Si-crystal. Angle of incidence  $\alpha = 0.1^\circ$ ; critical angle  $\alpha_{\text{crit}} \cong 0.15^\circ$ ,  $a_{\text{TF}} = 0.194 \text{ Å}$ . For the numerical integration of the equation of motion an average plane-potential has been used, which was derived from a Molière potential. The ordinate  $z$  gives the distance from the midplane of the crystal channel.

The trajectories in Fig. 1 were obtained by numerical integration of the equation of motion of 3 MeV protons, channeled between two neighboring (1, 1, 0)-planes of a Si-crystal.

In these calculations we used for the planar potential a Molière-potential averaged over the (1, 1, 0)-plane<sup>6</sup>

$$V(a) = 2\pi z Z e^2 D a_{\text{TF}} [(0.1/6) \exp(-6a/a_{\text{TF}}) + (0.55/1.2) \exp(-1.2a/a_{\text{TF}}) + (0.35/0.3) \exp(-0.3a/a_{\text{TF}})].$$

$a$  is the distance from the plane,  $ze$  and  $Ze$  are the charges of the projectile and the atoms in the plane, respectively;  $D$  is the planar density of the atoms in the (1, 1, 0)-crystal plane and  $a_{\text{TF}}$  means the Thomas-Fermi-screening distance which was chosen always as  $a_{\text{TF}} = 0.194 \text{ Å}$ . The wavelength of the trajectories shown is approximately 2000 Å. Due to the anharmonic potential used, the wavelengths of the trajectories are somewhat different, according to their different amplitudes. With an angle of incidence of  $\alpha = 0.1^\circ$  and 3 MeV proton energy, the

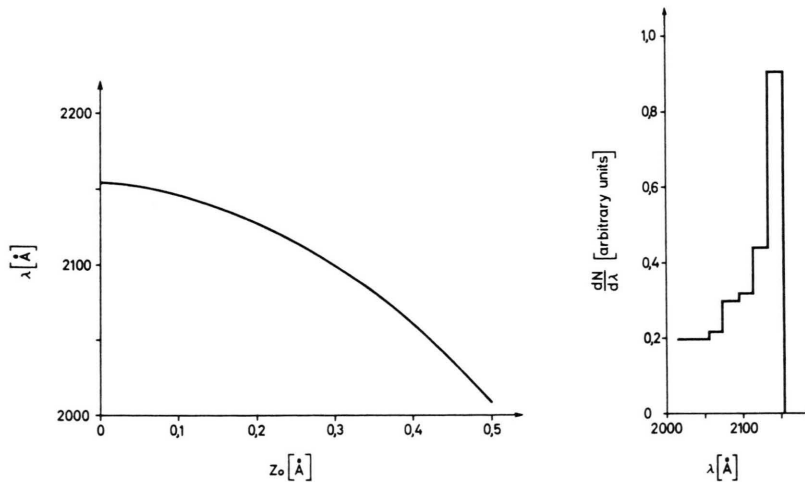


Fig. 2. a) Dependence of the wavelengths  $\lambda$  of the channeling trajectory on the ordinate  $z = z_0$  at the entrance into the crystal channel (same conditions as in Fig. 1).

b) Distribution of wavelengths ( $dN/d\lambda$ ) vs.  $\lambda$  (for the conditions of Fig. 1), i.e. relative number of trajectories with wavelengths  $\lambda$  within an interval  $\lambda \pm 10 \text{ Å}$  plotted as a function of  $\lambda$ .

<sup>6</sup> C. ERGINSOY, Phys. Rev. Letters **15**, 360 [1965].

wavelengths range from 2000 to 2150 Å. For this case, the dependence of the wavelength on the entrance  $z$ -coordinate  $z_0$  is given in Fig. 2a, and the spectrum of the wavelength  $\lambda$  in Fig. 2b, according to the calculations described below. The shortest wavelength is determined by our choice of  $a_{TF}$ , which limits the maximum amplitude. The energy loss of the transmitted particle is neglected in the calculations.

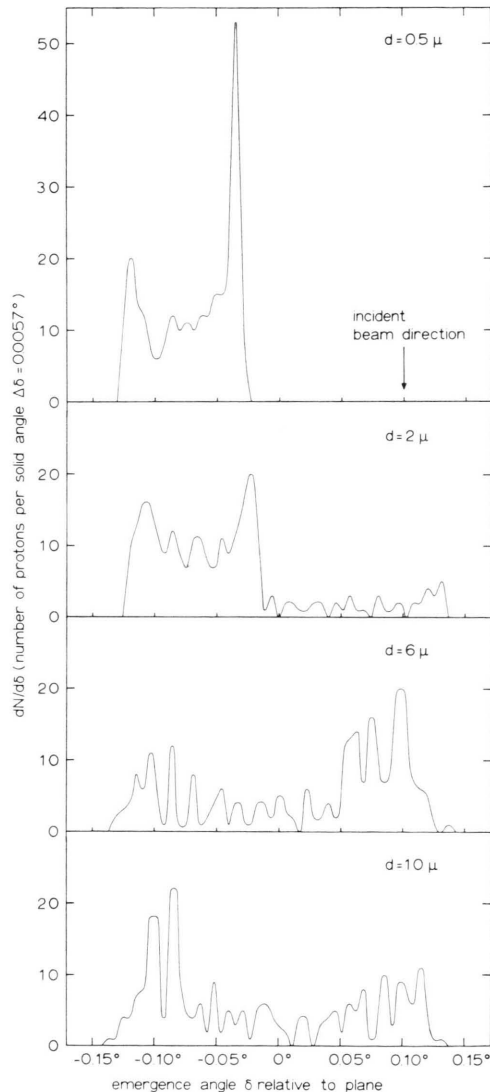


Fig. 3. Calculated angular distributions of coherently channeled 3 MeV protons, after the particles have left the (1, 1, 0)-planar channel. The four cases shown correspond to different channel lengths  $d$  (crystal thickness). A planar Molière potential  $V(a)$  was used. Energy losses were not taken into account.

In order to determine the angular distribution of coherently channeled particles, we calculated in each case 500 different trajectories starting all of them with the same angle of incidence  $\alpha$  with respect to the (1, 1, 0)-plane. The starting points between the planes at the entrance of the channel were equally spaced. Fig. 3 shows some results of these calculations for different thicknesses  $d$  of the crystal, i. e. different path lengths of the channeled particles. The angle of incidence was chosen to be  $\alpha = 0.1^\circ$ . The structure in the angular distributions is reproduced essentially in all details, if we used 1000 trajectories instead of 500.

The result of Fig. 3 with  $d = 0.5 \mu$  is at first sight somewhat surprising, since there is no intensity at angles  $0 \leq \delta \leq \alpha$ , whereas the whole intensity is located around  $\delta = -\alpha$ . Qualitatively, however this gross effect may be expected already from simple considerations if one realizes that  $d \cong 5\lambda/2$  and uses for illustration zig-zag-trajectories which give always a single intensity maximum at  $\delta = -\alpha$  for  $d = n\lambda/2$  ( $n$ : odd), and at  $\delta = \alpha$  for  $n$  being even. In addition to this gross structure, there is fine structure in the angular distribution due to details of the crystal potential.

In case of very thin crystals ( $0.5 \mu$ ,  $2 \mu$ , Fig. 3) which have thicknesses of up to about 10 average wavelengths  $\bar{\lambda}$  of the trajectories, two or three prominent fine structure peaks are obtained from the calculations besides other not so dominant structure.

With increasing crystal thickness  $d$ , the fine structure in the angular distribution gets more complicated with many peaks spaced at intervals of about  $0.02$ – $0.03^\circ$ . Averaging of this fine structure (as would occur with poor resolution) leads to a gross structure of broad peaks at  $\delta = \pm\alpha$  for the larger  $d$  values (Fig. 3). This can be understood qualitatively using the above mentioned simplified picture. We find, that the structure observed by EISEN<sup>7</sup> can be understood in terms of this calculated gross-structure.

For an experimental determination of the crystal potential, using fine structure measurements, it is important to know how sensitive this structure is with respect to variations of the potential. Our calculations show, that this sensitivity increases

<sup>7</sup> F. H. EISEN, Can. J. of Phys. **46**, 561 [1968] and Bull. Amer. Phys. Soc., Series II, **13**, No. 3402 [1968].

with increasing crystal thickness  $d$ . As an example, Fig. 4 shows an angular distribution for  $d = 10 \mu$ , the potential being increased only by  $\cong 3\%$  with respect to the original potential  $V(a)$  used for the

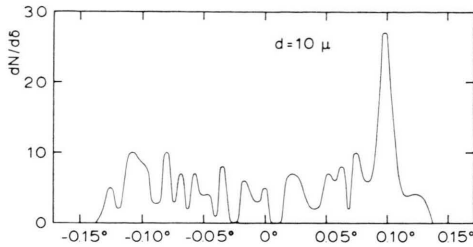


Fig. 4. Angular distribution of 3 MeV coherently channeled protons, assuming the same conditions as in Fig. 3 except that the planar Molière-potential was increased by  $\cong 3\%$ .

$10 \mu$  angular distribution calculation of Fig. 3. The two patterns are completely different, indicating therefore in this case a high sensitivity of the structure with respect to the crystal potential. In case of a  $0.5 \mu$  crystal (Fig. 3), however, the structure would have remained nearly the same except for a  $0.01^\circ$  displacement of the whole pattern.

The calculations discussed in this paper use a classical approach to the problem of coherent channeling, which seems to be most appropriate in our case as a first approximation. Nevertheless it should be mentioned, that quantum mechanical effects may

possibly modify our results to some extent. It may also be expected, from preliminary calculations, that temperature effects will smear out to some extent the fine structure, especially for larger crystal thicknesses.

### 3. Conclusions and Preliminary Experimental Results

According to our calculations, an experimental set up being able to detect the predicted structure in channeling lines of 3 MeV protons in Si must meet the following requirements (Fig. 3): the (thickness)-inhomogeneity of the crystal should be  $\leq 100 \text{ \AA}$  in the region used for channeling. The divergence of the incident beam as well as the angular resolution of the detector should be  $\leq 0.05^\circ$  for a  $0.5 \mu$  Si-crystal and  $\leq 0.02^\circ$  in case of  $10 \mu$  thickness. Preliminary experiments with an  $18 \mu$  thick single crystal of Si and an angular resolution and beam divergence of  $0.024^\circ$  have been performed by us at the Tandem-Van-de-Graaff Laboratory of the MPI Heidelberg.

The results<sup>8</sup> seem to show the predicted effects, i.e. we find fine structure for  $\alpha < \alpha_{\text{crit}}$ , which is not seen in the smooth angular distributions of channeled particles for  $\alpha \geq \alpha_{\text{crit}}$ . The main uncertainty in our results stems from the problem of making thin crystals with good enough thickness-homogeneity. A detailed account of the experiments will be given in a separate paper.

<sup>8</sup> C. MAYER-BOERICKE, M. ROGGE, and W. DUENNWEBER, Jahresbericht der KFA Juelich, 91, [1967].