

# Channelling of MeV H and He Ions in Alkali Halides at 'Zero Dose' Measurements

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## Abstract

Measurements of the minimum scattering yield  $\chi_{\min}$  and the half-angle for channelling  $\psi_{\frac{1}{2}}$  have been made for crystals of LiF, NaF, NaCl and KCl at very small total doses of  $\text{H}^+$  and  $^4\text{He}^+$  ions. The measured values of  $\psi_{\frac{1}{2}}$  are in good agreement with theory. Comparison of the results for  $\chi_{\min}$  as a function of depth, with theories based on a linear increase of the mean square beam divergence  $\Omega^2$ , shows that for the alkali halides studied the initial beam divergence  $\Omega_0$  on entering the crystal is proportional to  $\psi_1$ , the Lindhard characteristic channelling angle.

## 1. Introduction

With a well-collimated particle beam incident in a channelling direction on a crystal of good quality the probability of an atomic collision resulting in large-angle scattering is a minimum. A maximum amount of energy is dissipated in small-angle glancing collisions and electronic energy losses as the projectile ion passes down the channel. As lattice damage increases, the channels become less open and the chance of a collision leading to large-angle scattering correspondingly increases. Some lattice displacements occur in all such irradiation experiments but the rate of self-annealing of this lattice damage can differ considerably from substance to substance.

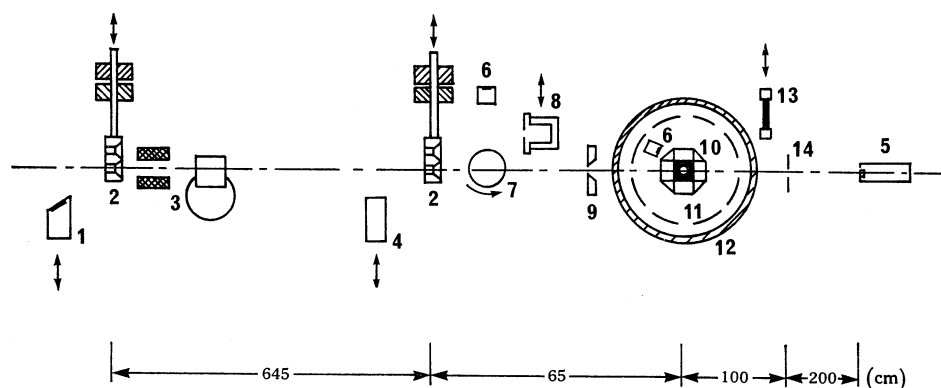
It has become evident from early channelling investigations that alkali halides exhibit an enhanced sensitivity to radiation damage from the measuring beam. This should be contrasted with the comparatively large dose tolerance of such crystals as tungsten and silicon, commonly used in channelling studies.

Some of the first evidence for this ready susceptibility of alkali halides came from measurements of the minimum scattering yield  $\chi_{\min}$  made by Matzke (1971). Very large  $\chi_{\min}$  values of from 0.15 to 0.40, were observed for various alkali halides with 1 MeV  $^4\text{He}^+$  ions. The high scattering values were blamed on the considerable amount of damage incurred during the alignment of the crystal, which was done using the particle beam. A saturation in the initial slope of aligned spectra (Morita *et al.* 1970) was observed at doses approaching  $1.5 \times 10^{14}$  ions  $\text{cm}^{-2}$  for 1.5 MeV protons on KBr. However, although a steep initial increase in the aligned slope was observed by Ozawa *et al.* (1972), no saturation was observed for doses up to  $1.5 \times 10^{15}$  ions  $\text{cm}^{-2}$  with 1.5 MeV protons. Recently, Hollis (1973) and Newton *et al.* (1976) found a recovery in  $\chi_{\min}$  with increasing dose for 1 MeV  $^4\text{He}^+$  ions on NaCl. The recovery was observed for doses between  $10^{15}$  and  $10^{16}$  ions  $\text{cm}^{-2}$ .

Besides the observations of the channelling half-angle  $\psi_{\frac{1}{2}}$  made by Matzke (1971), transmission measurements have been made for the  $\{100\}$  planes in a number of

alkali halides by Shipatov (1969) and Mannami *et al.* (1970). However, the number of measurements were comparatively few, the energies widely varied and the dose used unspecified. Because of the low current densities used in transmission experiments ( $10^{-6} \mu\text{A cm}^{-2}$ ), dose effects should be less than those for backscattered measurements.

The work described here and by Price (1973) is of measurements on various alkali halides of  $\psi_{\frac{1}{2}}$  and  $\chi_{\min}$  at as low doses as possible ('zero dose' measurements). The effect of increasing dose on  $\chi_{\min}$  and its variation with dose up to  $10^{17}$  ions  $\text{cm}^{-2}$  for both protons and  $\text{He}^+$  ions are discussed in a separate paper (Price and Kelly 1977).



**Fig. 1.** Channelling equipment: 1 and 4, beam viewers; 2, collimating apertures; 3, beam correcting magnet; 5, laser collinear with ion beam for crystal alignment; 6, surface barrier detectors; 7, rotating gold scattering vane as beam monitor; 8, Faraday cup for calibrating beam monitor; 9, antiscattering aperture; 10, goniometer; 11, liquid nitrogen cooled shield; 12, scattering chamber; 13, phosphor screen; 14, aperture and screen for laser alignment of crystal surface perpendicular to ion beam.

## 2. Experimental Method

### (a) Proton Measurements

Measurements with proton beams were made using the 3 MV Van de Graaff accelerator at the Australian Atomic Energy Commission, Lucas Heights. Beam collimation was by a 3 mm aperture followed at a distance of 645 cm by a 1 mm tantalum aperture. A 20 cm diameter eight-port scattering chamber was located with its centre 65 cm from the second aperture. The beam current was measured by means of a beam chopper placed immediately after the second aperture. The chopper was calibrated using a removable Faraday cup. Typical currents were 1–3 nA and the beam uniformity was checked before each aperture and after the goniometer (see Fig. 1).

Targets were mounted on a three-axis goniometer with an annular copper shield cooled to near liquid nitrogen temperatures.

### (b) $^4\text{He}^+$ Measurements

The results for 1 MeV  $^4\text{He}^+$  irradiations were obtained using the 2 MV Van de Graaff accelerator at the Australian National University, Canberra. In this case a three-circle Ortec goniometer surrounded by a liquid nitrogen cooled shield and centred in a 45 cm scattering chamber was used to orient the crystals. Beam

collimation was effected by means of a single square  $2 \times 2$  mm aperture immediately before the chamber, and the collimation was better than  $0.1^\circ$ .

The detection of backscattered particles, monitoring of beam current and mounting of targets were similar to those described above for the proton work, with the addition of a white light beam arranged to be collinear with the  $^4\text{He}^+$  beam, and introduced through a rear port on the analysing magnet. That part of the beam which passed through the target and a 1 mm aperture behind it was analysed using a Heath scanning monochromator EVE-700. A reference beam was provided by a polished stainless steel plate with a 1 cm aperture placed at  $45^\circ$  to the incident beam and before the collimating aperture. The reflected outer portion of the beam was monitored by a second monochromator.

### (c) Crystal Alignment

The ease and flatness with which common alkali halide crystals cleave normal to the  $\langle 100 \rangle$  axis enables them to be accurately aligned by reflection of a collimated light beam from this face (Price *et al.* 1973). Freshly cleaved Harshaw crystals were used in all experiments. In both experimental arrangements the reflection from a small helium-neon laser previously aligned with the incident beam was used to rapidly align the crystals to better than  $0.1^\circ$  with the  $\langle 100 \rangle$  axis without incurring the damage caused by the usual alignment procedure using the collimated particle beam.

### (d) Charge Neutralization

Since the targets are insulators, care was taken to minimize charging of the surface. For many of the proton irradiations, a small filament was mounted on the holder near the crystal. However, where the front clamping plate had a hole about 4 mm in diameter, as used for the  $^4\text{He}^+$  measurements, no evidence of serious surface charging was observed.

## 3. Theory

### (a) Monatomic Crystals

The interaction of well-collimated particle beams with aligned single crystals is characterized by two parameters, namely the minimum yield  $\chi_{\min}$ , normalized to that from a random distribution of the same atoms, and the critical angle  $\psi_c$ , an estimation of which is given by the half-width half-minimum  $\psi_{\frac{1}{2}}$  of the dip in the normalized scattering plotted as a function of incident angle. Lindhard (1965) has shown that estimates of  $\psi_{\frac{1}{2}}$  and  $\chi_{\min}$  may be obtained by treating the crystal as a series of 'strings' or rows of atoms whose average potential determines a characteristic angle  $\psi_1$ . The critical angle is related to  $\psi_1$  by

$$\psi_{\frac{1}{2}} = \alpha \psi_1, \quad (1)$$

where  $\alpha$  is a temperature-dependent parameter whose value has been calculated by Andersen (1967).

In the case of a monatomic row Lindhard (1965) has shown that

$$\psi_1 = (2Z_1 Z_2 e^2 / Ed)^{\frac{1}{2}} \quad \text{for} \quad \psi_1 \approx a_{\text{TF}} / d, \quad (2)$$

where  $Z_1$  and  $Z_2$  are the atomic numbers of the incident particles and target atoms

respectively,  $e$  is the electronic charge,  $E$  is the incident beam energy,  $d$  is the lattice spacing along the row and  $a_{\text{TF}}$  is the Thomas-Fermi radius. The corresponding expression for the planar case is (Picraux *et al.* 1969)

$$\psi_{\frac{1}{2}} = \beta(Z_1 Z_2 e^2 N d_p a_{\text{TF}}/E)^{\frac{1}{2}}, \quad (3)$$

where  $N$  is the atomic density,  $d_p$  is the spacing between planes and  $\beta$  is of order 1.

Using Monte Carlo computer calculations, Barrett (1971) has found that the expression

$$\psi_{\frac{1}{2}} = k F_{\text{RS}}(m u_1/a_{\text{TF}}) \psi_1, \quad (4)$$

with  $k = 0.8$  and  $m = 1.2$ , gives quite good agreement with a wide variety of experimental data. Here  $F_{\text{RS}}(\xi) = \{f_{\text{RS}}(\xi)\}^{\frac{1}{2}}$  with

$$f_{\text{RS}}(\xi) = \sum_{i=1}^3 a_i K_0(\beta_i \xi),$$

where  $K_0$  is the zero-order modified Bessel function and  $u_1 = \langle x^2 \rangle^{\frac{1}{2}} = \langle y^2 \rangle^{\frac{1}{2}} = \langle z^2 \rangle^{\frac{1}{2}}$  is the one-dimensional mean thermal vibration amplitude.

In the Lindhard (1965) formulation the minimum yield is given by

$$\chi_{\text{min}} = \pi N d (u_2^2 + a_{\text{TF}}^2) + \chi_3, \quad (5a)$$

where  $\chi_3$  is the contribution from amorphous surface layers and  $u_2 = \langle x^2 + y^2 \rangle^{\frac{1}{2}}$ ; the corresponding planar expression is

$$\chi_{\text{min}}(\text{planar}) = 2 a_{\text{TF}}/d_p. \quad (5b)$$

Barrett's (1971) calculations have indicated that a suitable expression is

$$\chi_{\text{min}} = \pi N d \{C(\Delta) u_2^2 + C'(\Delta) a_{\text{TF}}^2\}, \quad (6)$$

where  $\Delta$  is the variance of a gaussian distribution of beam directions. Since the quantity  $C'$  is about 0.2, a suitable approximation is given by

$$\chi_{\text{min}} = C(0) \pi N d u_2^2, \quad (7)$$

with  $C(0) = 3.0$ . An alternative expression (Picraux *et al.* 1969) for  $\chi_{\text{min}}$  is

$$\chi_{\text{min}} = \pi N d (\frac{1}{4} \pi a_{\text{TF}})^2 (\psi_1/\psi_{\frac{1}{2}})^4. \quad (8)$$

Here the effect of thermal vibrations is included through the measurements of  $\psi_{\frac{1}{2}}$ .

### (b) Extension to Polyatomic Crystals

Since the basis of Lindhard's (1965) theory of correlated scattering for atomic rows is a continuum potential based on an average of the periodic potential over the row direction, the extension of the theory to polyatomic crystals has generally consisted of using an average atomic number  $\bar{Z}_2$  for the row and an average lattice spacing  $\bar{d}$ . A similar method has been used for the planar case.

Gemmell and Mikkelsen (1972) have extended the formulae of Barrett (1971) to include polyatomic crystals. They have defined a critical angle for each type of row

or plane in terms of a summation of the static continuum potentials over each atomic species making up the row or plane. A similar treatment has been given for  $\chi_{\min}$ . While the calculated values for  $\psi_{\frac{1}{2}}$  were slightly lower than the experimental values when measured for BaTiO<sub>3</sub>, the calculated values for  $\chi_{\min}$  were approximately half those found experimentally.

An analytic form due to Varelas and Sizmann (1972) has been very successful in predicting values of  $\psi_{\frac{1}{2}}$  for equispaced rows with different atomic species and with similar atoms but unequal spacing. This method is based on applying the momentum approximation per periodic length of the row, rather than per atom as had been done previously.

**Table 1.** Comparison of predicted and experimental values of  $\psi_{\frac{1}{2}}$  and  $\alpha$

The calculated axial values for  $\psi_1$  and  $\alpha$  are from the Lindhard (1965) formula (2) and Fig. 5 of Andersen (1967) respectively; the calculated planar values for  $\psi_1$  and  $\psi_{\frac{1}{2}}$  are from equations (3) and (9)

Crystal	$E$ (MeV)	Calculated values			Experimental values		
		$\psi_1$	$\alpha$	$\psi_{\frac{1}{2}}$	$\psi_{\frac{1}{2}}^A$	$\alpha$	$\beta$
<i>(a) <math>\langle 100 \rangle</math> axial direction</i>							
NaCl	0.7	0.82°	0.90	0.74°	0.73°	0.89	
LiF	1.3	0.47	1.15	0.54	0.57 <sup>B</sup>	1.22	
NaF	0.8	0.67	1.08	0.72	0.67 <sup>B, C</sup>	1.00	
<i>(b) (100) planar direction</i>							
NaCl	0.7	0.14		0.26	0.20		1.4
NaF	0.8	0.14		0.26	0.23 <sup>B</sup>		1.6

<sup>A</sup> The experimental  $\psi_{\frac{1}{2}}$  values have a maximum error of about 10%.

<sup>B</sup> Values obtained by extrapolation of graphs of  $\psi_{\frac{1}{2}}(z)$  to  $z = 0$ .

<sup>C</sup> Value measured after a dose of  $2 \times 10^{15}$  ions cm<sup>-2</sup>.

#### 4. Results and Discussion

##### (a) 'Zero Dose' Measurements of $\psi_{\frac{1}{2}}$ and $\chi_{\min}$

We have measured  $\psi_{\frac{1}{2}}$  and  $\chi_{\min}$  for various alkali halides using the minimum possible dose. No attempt was made to obtain full dip curves, in order to minimize the damage introduced by the measurement. Because of this the number of points and the statistics for each point were severely limited. Similarly, since an increase in  $\chi_{\min}$  was observed by a dose of about  $5 \times 10^{13}$  H<sup>+</sup> cm<sup>-2</sup>, the statistics for the  $\chi_{\min}$  were not as good as could be desired.

The values of  $\psi_{\frac{1}{2}}$  measured for various alkali halides are given in Table 1 together with calculated values of  $\psi_1$ ,  $\alpha$  and hence  $\psi_{\frac{1}{2}}$ . The calculated value of  $\alpha$  was found from the curves of Fig. 5 of Anderson (1967) and  $\psi_1$  from Lindhard's (1965) equation (2) with  $Z_2 = \bar{Z}_2$ . Estimates of  $\psi_{\frac{1}{2}}$ (planar) were obtained both from Lindhard's approximation that the critical angle is

$$\psi_{\frac{1}{2}}(\text{planar}) \approx \frac{1}{2}(\bar{Z}_2)^{-1/6} \psi_1^*, \tag{9}$$

where  $\psi_1^*$  is given by the usual axial expression with a row spacing of  $\bar{d} = (d_p N)^{-1/2}$  and  $d_p$  the corresponding planar spacing, and also from equation (3) of Picraux *et al.* (1969). The calculated values of  $\psi_{\frac{1}{2}}$ (planar) in Table 1 were obtained from equation

(9), while values of  $\psi_1$  and  $\beta$  were obtained from equation (3) along with the measured values of  $\psi_{\frac{1}{2}}$ .

Where the spectra were suitable, extrapolations of  $\psi_{\frac{1}{2}}$  were made to  $z = 0$ . Examples of these extrapolations are shown in Fig. 2. The curves exhibit an upward trend as they approach the surface, similar to that observed by Campisano *et al.* (1972). For NaCl it is difficult to resolve the contributions from each element over any significant depth, although the protons scattered from the surface for each of the two ions are separated by about 30 keV and hence are just resolvable. We could thus obtain an estimate of  $\psi_{\frac{1}{2}}$  for  $z \approx 0$  by using the yield from the chlorine peak.

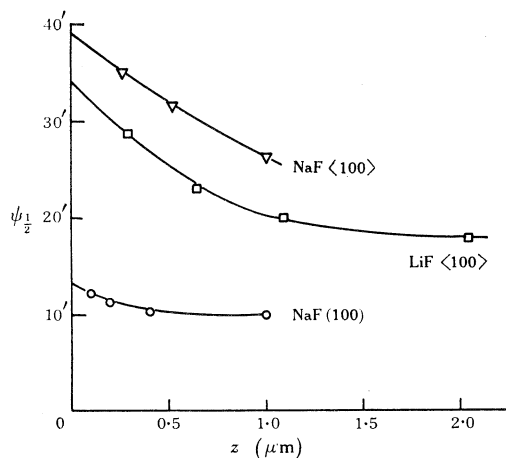


Fig. 2. Plots of the half-width  $\psi_{\frac{1}{2}}$  of the experimental channelling dip as a function of the depth  $z$  below the surface for  $\langle 100 \rangle$  axial channelling in NaF and LiF and (100) planar channelling in NaF.

In view of the limited dose that could be used to obtain the dip curves, the agreement shown in Table 1 between the experimental and predicted axial values of  $\psi_{\frac{1}{2}}$  is quite good. The result for NaF is somewhat low, as might be expected, following an incident dose of  $2 \times 10^{15}$  ions  $\text{cm}^{-2}$ . Agreement with the Lindhard approximation is fair for the planar measurements, being better for NaF than NaCl. However, the values of  $\beta$  required for equation (3) are much greater than those originally suggested.

Comparison of the present results with those of earlier workers indicates some differences. In a transmission experiment with 1.5 MeV protons, Mannami *et al.* (1970) obtained a value of  $0.25^\circ \pm 0.04^\circ$  for the (100) planar critical angle for NaCl. This angle is larger than that measured here yet the energy was greater than in the present work by just over a factor of two.

Reasonable agreement between the planar measurements of  $\psi_{\frac{1}{2}}$  for a number of alkali halides (NaCl, KCl, KBr and KI) and a simple estimate based on the minimum distance of approach taken as  $a_{\text{TF}}$  were obtained by Mannami *et al.* (1970). They made two estimates for each based on  $a_{\text{TF}}$  for either the positive or negative ion. The poorest agreement occurred for NaCl.

We have estimated the critical angle for NaCl and NaF from calculations of the static average  $\langle 100 \rangle$  row and (100) planar potentials from average potentials given by Appleton *et al.* (1967). Average values of  $Z_2$  and  $d$  were used for all calculations including the Thomas-Fermi radii. Values of the zero-order modified Bessel function  $K_0(x)$  required for the potential calculations were taken from Abramowitz

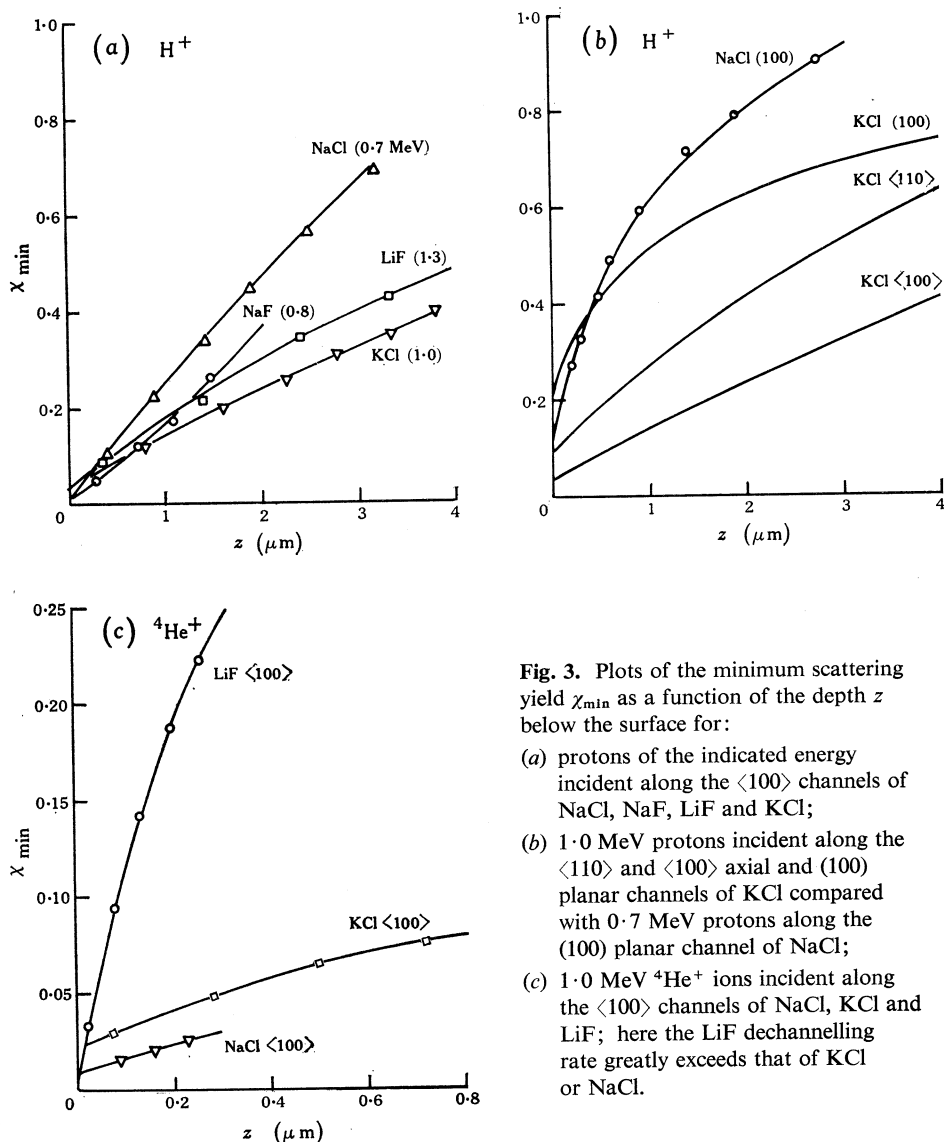


Fig. 3. Plots of the minimum scattering yield  $\chi_{\min}$  as a function of the depth  $z$  below the surface for:

- protons of the indicated energy incident along the  $\langle 100 \rangle$  channels of NaCl, NaF, LiF and KCl;
- 1.0 MeV protons incident along the  $\langle 110 \rangle$  and  $\langle 100 \rangle$  axial and (100) planar channels of KCl compared with 0.7 MeV protons along the (100) planar channel of NaCl;
- 1.0 MeV  $^4\text{He}^+$  ions incident along the  $\langle 100 \rangle$  channels of NaCl, KCl and LiF; here the LiF dechannelling rate greatly exceeds that of KCl or NaCl.

and Stegun (1966). Values of  $\psi_{\frac{1}{2}}$  were then calculated from

$$E\psi_{\frac{1}{2}}^2 = U(r_{\min}), \quad (10)$$

with  $r_{\min} = a_{\text{TF}}$ . Estimates of  $r_{\min}$  were obtained by using the measured critical angles. Generally the agreement between the measured and calculated values of  $\psi_{\frac{1}{2}}$  and hence  $r_{\min}$  and  $a_{\text{TF}}$  was fair. However, a large discrepancy was found in the case of (100) NaCl.

Measurements of  $\chi_{\min}$  and  $\psi_{\frac{1}{2}}$  by Matzke (1971) gave very large values for  $\chi_{\min}$  (about an order of magnitude greater than predicted) with a corresponding smaller value for  $\psi_{\frac{1}{2}}$ , which was attributed to damage due to the incident beam. Agreement

with the present results is good for NaCl but for LiF Matzke's value of  $\alpha = 0.92 \pm 0.08$  is to be compared with our result of  $1.22 \pm 0.1$ . The difference is believed to be directly attributable to the large but unknown amount of damage caused by the beam in the earlier experiments.

Curves for  $\chi_{\min}$  as a function of depth  $z$  are shown in Figs 3*a*–3*c* for both the  $\text{H}^+$  and  $^4\text{He}^+$  beams. From the  $\langle 100 \rangle$  measurements with protons (Fig. 3*a*) it can be seen that the slopes of the yield curves may be divided into two sets: (1) NaCl and NaF and (2) LiF and KCl. A similar smaller dechannelling rate for KCl (100) than for NaCl (100) is observed in Fig. 3*b*, which also shows a progressive increase in dechannelling rate from the  $\langle 100 \rangle$  to the  $\langle 110 \rangle$  and (100) directions for KCl.

The lower dechannelling rate for  $\text{H}^+$  in LiF shown in Fig. 3*a* should be contrasted with the curve for  $^4\text{He}^+$  in LiF shown in Fig. 3*c*, where the dechannelling rate for LiF is much greater than for either NaCl or KCl.

Table 2. Comparison of predicted and experimental values of  $\chi_{\min}$

The calculated axial values for  $\chi_{\min}$  are from the Lindhard (1965) formula (5*a*), the Barrett (1971) formula (6) and the Picraux *et al.* (1969) formula (8); the calculated planar values for  $\chi_{\min}$  are from equation (5*b*)

Crystal	Ion	Calc. $\chi_{\min}$ (eqn 5a)			Calc. $\chi_{\min}$ (eqn 6)		Calc. $\chi_{\min}$ (eqn 8)	Exp. $\chi_{\min}$
		$\pi Nd \times u_2^2$	$\pi Nd \times a_{\text{TF}}^2$	$\pi Nd \times (u_2^2 + a_{\text{TF}}^2)$	$C = 3, C' = 0.2$	$C = 3, C' = 0$		
(a) $\langle 100 \rangle$ axial direction								
KCl	H <sup>+</sup>	0.014	0.008	0.022	0.044	0.042		0.04
	<sup>4</sup> He <sup>+</sup>	0.014	0.008	0.022	0.044	0.042		0.02
NaCl	H <sup>+</sup>	0.015	0.012	0.027	0.048	0.046	0.012	0.015
	<sup>4</sup> He <sup>+</sup>	0.015	0.012	0.027	0.048	0.046		0.01
NaF	H <sup>+</sup>	0.012	0.021	0.033	0.040	0.036	0.006	0.01
LiF	H <sup>+</sup>	0.013	0.039	0.052	0.047	0.039	0.006	0.04
	<sup>4</sup> He <sup>+</sup>	0.013	0.034	0.047	0.045	0.039		0.01
(b) $\langle 110 \rangle$ axial direction								
KCl	H <sup>+</sup>	0.020	0.012	0.032	0.062	0.060		0.09
(c) (100) planar direction								
KCl	H <sup>+</sup>						0.11	0.22
NaCl	H <sup>+</sup>						0.13	0.11

Surface values of  $\chi_{\min}(z)$  may be obtained by extrapolation of curves of  $\chi_{\min}$  versus depth such as those in Fig. 3. For comparison with these results, we have calculated values for axial directions from the Lindhard (1965) formula (5*a*) in Section 3 above (with  $\chi_3 = 0$ ), from the Barrett (1971) formula (6) (with  $C = 3$  and both  $C' = 0.2$  and 0) and, where the critical angle was measured, from the Picraux *et al.* (1969) formula (8). Planar values have been compared with the expression (5*b*) for a static lattice from Davies *et al.* (1968). Along with the extrapolated experimental results, all these calculated values are shown in Table 2. In general the agreement between theory and experiment is good.



For very small values of  $\chi_{\min}$  ( $\approx 0.01$ ) the absolute error in the extrapolation could give rise to errors of 25–50 % in the case of the proton yields. However, this would not be sufficient to account for the magnitude by which  $\chi_{\min}(\text{exp.})$  is less than  $\chi_{\min}(\text{theor.})$  for NaCl and NaF when the results are compared with Barrett's (1971) formula. For all the crystals except LiF, we have  $a_{\text{TF}}^2 \approx u_2^2$  and the sum of these two terms used in Lindhard's (1965) expression agrees fairly well with the results for NaCl and NaF, while the observed result for KCl is anomalously high. For LiF, we have  $a_{\text{TF}}^2 > u_2^2$  and the Lindhard expression with only  $a_{\text{TF}}$  is probably the more correct.

Only static lattice estimates have been made for (100) proton minimum yields from KCl and NaCl. Agreement with the results is good for NaCl but not at all so for KCl. Similarly there is a discrepancy between the predicted and observed results for the  $\langle 110 \rangle$  axis for KCl. The  $\langle 110 \rangle$  result should only differ from the  $\langle 100 \rangle$  result by the ratio  $d_{\langle 110 \rangle}/d_{\langle 100 \rangle} = 1.41$  whereas the observed ratio is 2.25. It is possible, though unlikely, that the crystal was consistently slightly misaligned to this extent in each of the three KCl observations but not in any of the other experiments.

(b) *Relation between Initial Beam Divergence and  $\psi_1$*

Normalized yields for a number of the backscattered spectra have been compared with the simple theory of Ellegaard and Lassen (1967), as extended by Fujimoto *et al.* (1971) to include beam divergence and surface effects. The theory predicts an expression for  $\chi_{\min}(z)$  of the form

$$\chi_{\min}(z) = \chi_{\min}(0) + \{1 - \chi_{\min}(0)\} \exp(-L/z), \quad (11)$$

where  $L$  is the depth for the mean scattering angle  $\Omega$  to be equal to the critical angle  $\psi_c$  for channelling; that is, we have the relation

$$\Omega^2 = (\psi_c^2/L)z, \quad (12)$$

and generally

$$\psi_c \approx \psi_1 = (2Z_1 Z_2 e^2/Ed)^{\frac{1}{2}}.$$

However, the results have usually been plotted in terms of  $E^1$ , the energy difference between particles scattered below the surface and those scattered from the surface, and the ratio  $\xi = z/L$ , which from equation (11) is given by

$$\xi = \left\{ \ln \left( \frac{1 - \chi_{\min}(0)}{\chi_{\min}(E^1) - \chi_{\min}(0)} \right) \right\}^{-1}. \quad (13)$$

In all cases the graphs of  $\xi$  versus  $E^1$  have been linear up to values of  $\xi \approx 1$ . Because of the generally nonlinear relationship between the depth of scattering  $z$  and the emitted energy  $E$  at the surface, these linear fits for  $\xi(E^1)$  are somewhat disturbing. The difficulty is increased by an inability to ascribe a unique depth (within the limits set by straggling) to the scattered particles since the stopping power for channelled particles is impact-parameter dependent. However, for depths for which  $\xi \lesssim 1$  the variation in random stopping with depth is quite small.

Plots of  $\xi$  versus  $z$  for four alkali halides are shown in Fig. 4. Although the energies for the various curves are different in each case, the singularly interesting

feature of the plots is the fact that the extrapolated curves all have the same value at  $z = 0$ . Except for NaF, the curves are linear up to  $\xi \approx 1$  with the fits for KCl and LiF being particularly good.

The distance  $l_n$  corresponding to an increase in the mean scattering angle equal to  $\psi_1$  in a random material is given by Lindhard (1965) as

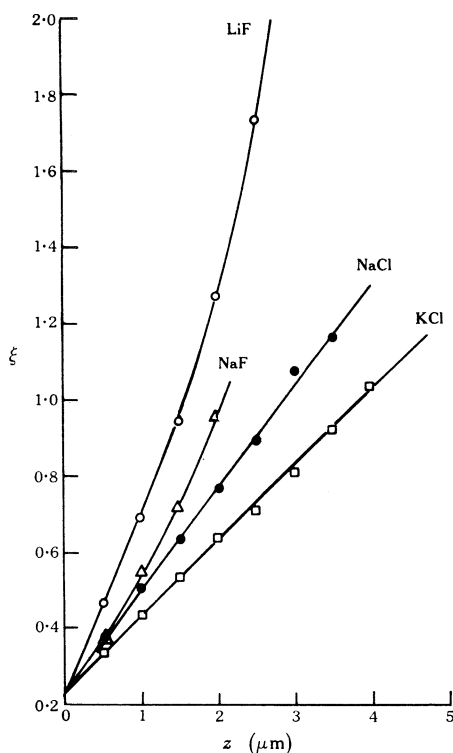
$$l_n = 2/\pi Nd^2 L_n \psi_1^2,$$

where

$$L_n = \ln\{1 \cdot 29(a_{TF} E M_2 / Z_1 Z_2 e^2 (M_1 + M_2))\},$$

$M_1$  and  $M_2$  being the rest mass of the projectile and target atom respectively. A dechannelling coefficient  $\gamma$  may then be defined as

$$\gamma = l_n / L.$$



**Fig. 4.** Plots of the ratio  $\xi$  (defined by equation 13) as a function of the depth  $z$  below the surface for protons incident along the  $\langle 100 \rangle$  channels of LiF, NaF, NaCl and KCl. Except for NaF, the fitted curves are linear up to  $\xi \approx 1$ .

Values for the initial beam divergence  $\Omega_0$  may also be obtained from the approximate expression based on Lindhard's standard potential (Fujimoto *et al.* 1971)

$$\Omega_0^2 = 3(a_{TF}/a_0)^2 \psi_1^2,$$

where  $a_0 = (\pi Nd)^{-\frac{1}{2}}$ . Observed values of  $l_n$ ,  $L$  and hence  $\gamma$  along with observed and calculated values of  $\Omega_0$  are shown in Table 3 for the LiF, NaCl and KCl curves of Fig. 3a. For comparison, in the last row are listed values obtained by Fujimoto *et al.* (1971) for 1.5 MeV protons on KCl.

All the observed values of  $\gamma$  listed in Table 3 are much higher than that given by Fujimoto *et al.* (1971). The change in energy from 1.5 to 1.0 MeV would be

expected to reduce  $\gamma$  through the  $\psi_1^2$  term in  $l_n$  in the opposite direction to the observed value. However, the discrepancy may be partly accounted for by the choice of the parameter  $\beta$ . Fujimoto *et al.* (1971) used a value of  $\beta = 0.45$  whereas the depth scales in Fig. 3 were derived using  $\beta = 1$ . This would result in an extension of our depth scale leading to a smaller estimated value of  $L$  and hence a larger value of  $\gamma$ . In view of the results of Edge and Dixon (1970) and the decision at Aarhus (see Davies *et al.* 1972), it would appear that our higher value is the better one to use.

Table 3. Observed values of channelling parameters

Crystal	$E$ (MeV)	$l_n$ ( $\mu\text{m}$ )	$L$ ( $\mu\text{m}$ )	$\gamma$	Obs. $\Omega_0$ (mrad)	Calc. $\Omega_0$ (mrad)
LiF	1.3	0.236	3.77	0.063	3.98	2.79
NaCl	0.7	0.104	2.11	0.049	7.10	2.81
KCl	1.0	0.181	5.06	0.036	6.30	2.08
KCl <sup>A</sup>	1.5	0.253	—	0.0189	3.7	1.8

<sup>A</sup> Values from Fujimoto *et al.* (1971) for comparison.

It appears to be quite remarkable, in view of the variation of energy and sample, that the crossing points of plots of  $\xi$  versus  $z$  should, as noted above, all intersect at the same  $\xi$  value at  $z = 0$ . The implication is that values of  $\Delta z/L = (\Omega_0/\psi_1)^2$  are independent of the crystal type and energy, or much less probably that there is a compensating variation of these two factors in the present results. Fujimoto *et al.* (1971, 1972) have observed a similar intersection of the  $\xi$ - $z$  curves both for various temperatures in germanium and at increasing doses and hence damage in KCl; the latter observation indicating that  $\Omega_0$  is independent of crystal imperfections, the former indicating that equation (13) holds for the region where the beam divergence is less than the critical angle. In the above case if  $\Omega_0^2$  is to depend only on  $\psi_1^2$  then it must depend on  $\bar{Z}_2$ ,  $E$  and  $d$  in a similar manner.

Since for those particles that are dechannelled comparatively close to the surface, i.e. at depths for which  $\xi < 1$ , the major dechanneling mechanism is nuclear scattering, as these will be the particles with the highest initial transverse energy. Following Bohr (1948) we can write for particles with an initial energy  $E_0$

$$\left(\frac{d\Omega^2}{dx}\right)_n = \frac{M_2}{M_1 E_0} \left(-\frac{dE}{dx}\right)_n \quad (14)$$

and this gives

$$\Omega^2 \propto \Delta E,$$

where  $\Omega^2$  is the mean square scattering angle for an energy loss  $\Delta E$ . Calculations of the emitted energy for particles scattered at increasing depths in the alkali halide crystals used here show that in the case of random stopping (and probably for aligned spectra) the variation is very nearly linear for small depths:  $\lesssim 2 \mu\text{m}$  for NaCl (0.7 MeV) and NaF (0.8 MeV) and somewhat better for LiF (1.3 MeV) and KCl (1.0 MeV). Thus it is possible to write  $\Omega^2 \propto E^1$ .

The fact that  $\xi = 0.24$  for  $E^1 = 0$  implies that  $\xi = (z + \Delta z)/L$  in equation (13) or, in terms of  $E^1$ , that  $\Delta E^1/E^1 = \text{const.}$  and  $\Omega_0^2 \propto \psi_c^2$ . Since  $\psi_c \approx \psi_1$  we thus have  $\Omega_0^2 \propto \psi_1^2$ .

## 5. Conclusions

By keeping the dose per point as low as possible we have obtained values for  $\psi_{\frac{1}{2}}$  and  $\chi_{\min}$  that show comparatively good agreement with theory; the results for  $\psi_{\frac{1}{2}}$  being better than those for  $\chi_{\min}$ . Some of the  $\chi_{\min}$  values are quite small (0.01–0.02) and these may reflect the poor statistics involved. However, it should be pointed out in defence of our results that freshly cleaved crystals gave very little evidence of a surface peak, a behaviour which is consistent with a low  $\chi_{\min}$ .

For values of  $\xi \lesssim 1$  (equation 13) generally good fits have been obtained to the aligned backscattered spectra for various alkali halides and energies. Values of  $\Omega_0$  have been found to be consistently higher than those predicted using the expression due to Fujimoto *et al.* (1971). A similar observation was made by Fujimoto *et al.* in the case of KCl. In the region up to  $\xi = 1$  there is essentially a linear relation between  $E^1$  and  $z$  (we have also found this for silicon for 1.5 MeV protons) which explains the anomaly noted by Fujimoto *et al.* The fact that all the axial proton measurements have the same value of  $\xi$  at the surface can be used to show that the initial mean scattering angle of the beam on entering the crystal is proportional to  $\psi_1$ .

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