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Diffraction of X-rays by the Faulted Cylindrical Lattice of Chrysotile. II. The Form, Position and Width of some Diffraction Profiles

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The measurements of the form, position and half-height width of some important reflexions were carried out on 15 chrysotile fibres from different localities. The samples do not differ significantly in length of reciprocal lattice parameters a^*, b^*, mean diameter of cylindrical lattice and wall thickness. We found for these characteristics the following average values: $a^* = 0{\cdot}06855$ Å, $b^* = 0{\cdot}10860$ Å, the mean diameter 234 Å, and the wall thickness 155 Å. The samples differ significantly in the different degree of axial disorder present in the cylindrical lattice.

Introduction

In this paper, which is a direct continuation of our first paper (Toman & Frueh, 1968), hereinafter referred to as TF1, we describe our experimental work on chrysotile fibres of different origins, and give our results concerning the form, position and half-height width of some important profiles. A list of the fibres studied in this paper is given in Table 1. The chemical composition of fibre No. 15 is indicated in the paper of Hodgson (1967); the exact composition of the remaining fibres is not known. The tensile strengths of the fibres is shown in the last column of Table 1. The tensile tests were made by Mr A. Winer of the Canadian Department of Energy, Mines and Resources, using a table model Instron Tester. Tension cell B with a range of 0 to 2000 grams was used, and the cross-head speed and chart speed used were 0·01 in.min^{-1} and 1 in.min^{-1} respectively. Only tests that showed a clean break of the fibre were utilized.

Apparatus

The distribution of the diffracted intensity of Cu $K\alpha$ radiation was measured by using a counter diffractometer of the equi-inclination type. As detector of radiation, a proportional counter was used. The influence of unwanted radiation was minimized by using an electronic amplitude analyser and a balanced-filter technique. Parallel bundles of chrysotile fibres, having an outside diameter of 0·1–0·2 mm, were used as samples. During the exposure they were fixed in a special holder under slight tension.

Careful attention was paid to the exact orientation and centring of our specimens on the diffractometer. The orientation of the equatorial plane of the reciprocal lattice of the fibre onto the equatorial plane of the diffractometer was accomplished in the standard way by bringing the reflexion 060 into the equatorial plane of the diffractometer for four different orientations of the fibre, differing by 90° around the ω axis.

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Table 1. *List of samples, their localities and tensile strengths*

Sample No.	Locality	Mean tensile strength $\times 10^{-5}$ (lb. in^{-2})
1	Jeffrey Mine, Asbestos, P.Q.	4·2
2	King Beaver Mine, Thetford Mines, P.Q.	3·0
3	Normandie Mine, Vimy Ridge, P.Q.	1·7
4	Bell Mine, Thetford Mines, P.Q.	2·9
5	Lake Asbestos A, Black Lake, P.Q.	2·3
6	Lake Asbestos B, Black Lake, P.Q.	3·7
7	Lake Asbestos C, Black Lake, P.Q.	3·4
8	Cassiar Asbestos, Cassiar, B.C.	2·9
9	Barraba No. 2, Barraba, N.S.W., Australia	0·8
10	Barraba No. 4, Barraba, N.S.W., Australia	1·4
11	Barraba No. 6, Barraba, N.S.W., Australia	1·6
12	Russian AK-2, USSR	2·6
13	Gilla County, Arizona	5·0
14	Johnson's Mine, Thetford Mines, P.Q.	3·3
15	King Beaver Mine, Thetford Mines, P.Q.	5·3

For this, an entrance slit 0·3° wide, parallel with the equatorial plane of the diffractometer, was used. The centring of the fibre was performed in such a way that the 2θ angle of the 400 reflexion was constant within 0·1° for any orientation of the fibre around the ω axis. For the centring of the fibre we used the 0·1°-wide entrance slit parallel to the fibre. Insufficient accuracy in the alignment of the fibre caused considerable dependence of the width of the diffraction profiles on the orientation of the fibre around the ω axis. The collimator used in all work had a circular opening 0·25 mm in diameter.

Because the main aim in this work lies in the exact measurement of the form and width of the diffraction profile, we considered it important to estimate the extent of instrumental distortion inherent in our apparatus. For this reason we measured the line width of the 200 reflexion of an annealed copper wire 0·15 mm in diameter. The width of the 200 maximum in its half-height was 0·32°, which corresponds to 0·0035 $Å^{-1}$. We were not able to reduce this relatively unfavourable value of the instrumental broadening without suffering a marked loss in intensity. As will be seen further, the measured profiles were not narrower than 0·006 $Å^{-1}$, and therefore we felt justified in accepting this relatively poor resolving power.

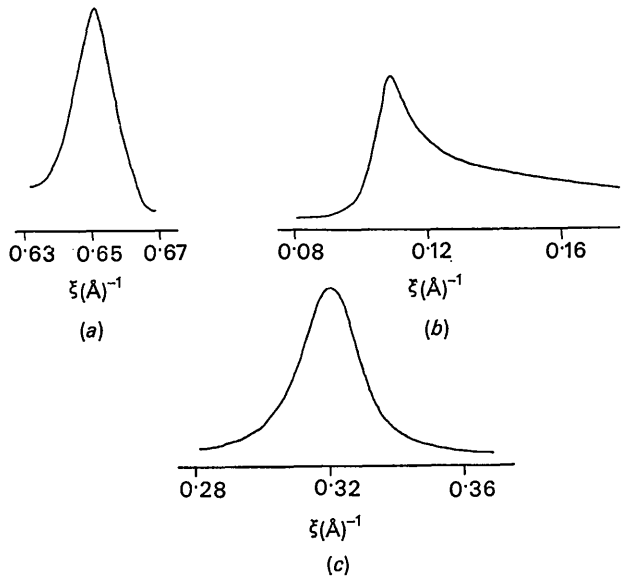

Fig. 1. Diffraction profiles of (*a*) 060, (*b*) 011 and (*c*) 033 from sample 6.

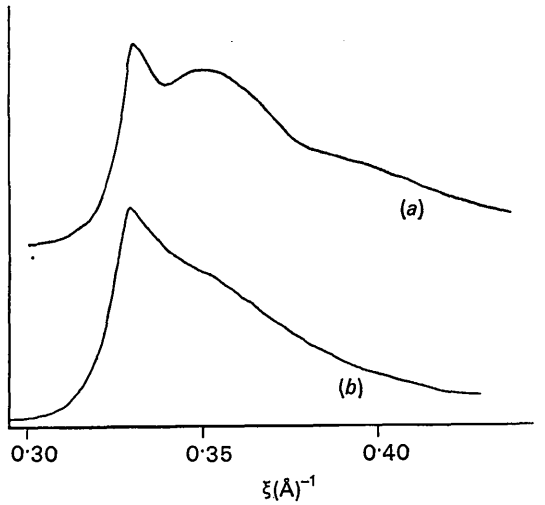

Fig. 2. Diffraction profiles of 031 from (*a*) sample 7 and (*b*) sample 13.

The form of the reflexions

We measured the form both of the *h*0*l* reflexions (which are determined mainly by terms containing zero-order Bessel functions) and of the 0*kl* reflexions (which are determined by terms containing high-order Bessel functions; see TF1). Reflexions 200, 400 and 202 were found to be symmetrical, as expected from the theory. Reflexions 060, 011 and 033 have a similar form for all samples measured, and differ among themselves only in their width. They are asymmetrical and their form corresponds closely to the form of computed profiles, calculated in TF1 for the case of the model with the maximum number of cylindrical azimuthal boundaries (Fig. 1). This means that in this model every silica–brucite double layer is independent from the point of azimuthal displacements, and has such a number of unit cells per unit angle as to insure the minimum strain in every mosaic block (double layer) – the model first introduced by Whittaker (1957).

The profile of the reflexion 031 does not conform with this supposition. Most samples display a profile with two maxima, which does not correspond to the model with the maximum number of cylindrical azimuthal boundaries, but rather to a model with a lower number, such as was used in TF1 to compute the distribution shown in Fig. 5(*b*) of that paper. Only sample 13 gives a profile of reflexion 031 with only one maximum, corresponding more closely to the profile expected for Whittaker's model (Fig. 2).

However, it does not seem to us that there is enough evidence to abandon Whittaker's model in favor of some more complicated structure of cylindrical azimuthal boundaries. Therefore, all our further interpretations of the line width are based on acceptance of Whittaker's model.

The position of reflexions

We measured the positions of the maxima (the radial cylindrical coordinate ξ_{max}) for reflexions 200, 400, 060, 011 and 033. The measurement was always performed for two orientations of the fibre (with respect to rotation around the ω axis by 180°). In Table 2 the mean of these two readings is shown (columns 2–6).

The results shown in columns 2–6 of Table 2 are supposedly influenced by two kinds of systematic error,

as well as by random errors. One of them is here referred to as Δ, the shift of the zero of the ω scale (due to the imperfect alignment of the diffractometer), which is constant for all samples and all reflexions. The other is denoted as p, the shift of the position of the reflexion due to the imperfect centring of the sample (for our limited range $\theta < 35°$). We assume that p is approximately the same for different reflexions on a certain layer line of the same sample, but differs in a random way from sample to sample. Clearly, the difference $\xi_{400} - \xi_{200}$ (column 7) is influenced neither by Δ nor by p; it is subjected only to random errors. The difference $\xi'_{200} - \xi_{200}$, denoted here as K (column 17), is a correction constant allowing for Δ and p, but including cumulated random errors from ξ_{200} and ξ_{400}. Using K we got corrected values ξ'_{max} for 060, 011 and 033 reflexions (columns 7, 10, 11). The corrected value ξ'_{max} for 400 is not an independent value because it is exactly twice the ξ'_{max} value for the 200 reflexion. K is a more useful correction factor for the reflexions on the equator because it was derived on the basis of equatorial reflexions. When applied to the reflexions on the higher layer lines, it properly corrects only the error induced by Δ, and inadequately corrects the errors caused by p (which are assumed to be different for different layer lines) and, in addition, it accumulates larger random errors. For this reason, we introduce the correction constant Δ', the average value of K over all fibres measured, which corrects only for the shift Δ and is supposed to be virtually free of random errors. The radial reciprocal coordinates corrected by Δ' are denoted as ξ''_{max} (columns 12–16); the value of Δ' is 37×10^{-4} Å^{-1}, and its r.m.s. deviation $4{\cdot}8 \times 10^{-4}$ Å^{-1}.

In Table 3 we show the mean values and the r.m.s. deviations of all radial reciprocal coordinates from Table 2.

From Table 3 we can see the merits of using corrections K and Δ' respectively. The r.m.s. deviations of ξ'_{max} for the 200 and 600 reflexions are lower than those of the uncorrected ξ'_{max}. This reflects the fact that the errors Δ and p are properly allowed for. On the other hand, the r.m.s. deviations of ξ' for the 011 and 033 reflexions are higher than those of uncorrected ξ_{max} for these reflexions. This can be expected, because only the error Δ is corrected satisfactorily, and a large accumulated random error is introduced. The r.m.s. deviations of ξ''_{max} (corrected by using the constant Δ') are the same as those of the uncorrected set, because the correction is the same for the entire set.

Now we need to have some idea how large a part of the r.m.s. deviations of the radial reciprocal coordinates of the reflexions is due to errors of measurement, and what can be considered the result of differences in the structure of the cylindrical lattice of individual samples. For this reason a series of 10 independent measurements was made of the position of reflexions 200, 011 and 033 with the same fibre, no. 6, in such a way that before every measurement the fibre was misaligned and then oriented and centred over again. Results are summarized in Table 4.

If we compare the r.m.s. deviations in Table 2 with those in Table 4, it appears that the differences in the

Table 2. *The uncorrected* (ξ_{max}) *and corrected* (ξ'_{max}, ξ''_{max}) *radial reciprocal coordinates of reflexions and the correction constant K*

Sample No.	$10^4\,\xi_{max}$ Uncorrected (Å^{-1})					$10^4\,\xi_{max}'$ Corrected using K(Å^{-1})					$10^4\,\xi_{max}''$ Corrected using Δ (Å^{-1})					10^4K (Å^{-1})
	200	400	060	011	033	200	400*	060	011	033	200	400	060	011	033	
(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)	(9)	(10)	(11)	(12)	(13)	(14)	(15)	(16)	(17)
1	1336	2708	6497	1100	—	1372	2744	6533	1136	—	1373	2745	6534	1137	—	36
2	1340	2705	6497	1100	3239	1365	2730	6522	1125	3264	1377	2742	6534	1137	3276	25
3	1330	2702	6490	1103	3224	1372	2744	6532	1145	3266	1367	2739	6527	1140	3261	42
4	1333	2701	6485	1102	3248	1368	2736	6520	1137	3283	1370	2738	6522	1139	3285	35
5	1334	2707	6497	1105	3239	1373	2746	6536	1144	3278	1371	2744	6534	1142	3276	39
6	1333	2705	6488	1115	3229	1372	2744	6527	1154	3268	1370	2742	6525	1152	3266	39
7	1335	2704	6490	1105	3242	1369	2739	6524	1139	3277	1372	2741	6527	1142	3279	34
8	1333	2705	6486	1110	3245	1372	2744	6525	1149	3284	1370	2742	6523	1147	3282	39
9	1340	2710	6495	1104	3218	1370	2740	6525	1134	3248	1377	2747	6532	1141	3255	30
10	1333	2702	6493	1097	3227	1369	2738	6529	1133	3263	1370	2739	6530	1134	3264	36
11	1332	2705	6485	1100	3224	1373	2746	6526	1141	3265	1369	2742	6522	1137	3251	41
12	1338	2710	6486	1113	3238	1372	2744	6520	1147	3272	1375	2747	6523	1150	3275	34
13	1330	2700	6476	1111	3257	1370	2740	6516	1151	3297	1367	2737	6513	1148	3294	40
14	1330	2714	6480	1104	3242	1374	2748	6524	1148	3286	1367	2741	6517	1141	3279	44
15	1330	2702	6487	1094	3250	1372	2744	6529	1136	3292	1367	2739	6524	1133	3287	42

* Depends upon ξ_{max}' for 200 reflexion.

Table 3. *The mean values and r.m.s. deviations of radial reciprocal coordinates of measured reflexions*

	Uncorrected					Corrected using K					Corrected using Δ'				
Mean	200	400	060	011	033	200	400	060	011	033	200	400	060	011	033
$10^4\xi$	1334	2705	6489	1104	3237	1371	2792	6526	1141	3274	1371	2742	6526	1141	3274
$10^4\sigma_\xi$	3·3	3·0	6·0	5·2	10·9	2·3	—	5·2	7·5	12·8	The same as for uncorrected				

ξ_{200} can be explained by random errors of measurement, so we assume that all our samples exhibit the same dimension a^* of the reciprocal lattice within the limits of accuracy of our measurements. The same is true with reflexions 011 and 033, which are rather important because on the basis of ξ_{011} and ξ_{033} we are able to determine the mean radius of the cylindrical lattice (see TF1). Even here, all measurements lie within the limits of errors, as indicated by Table 4. This point can be confirmed by examining the correlation coefficient r for ξ_{011} and ξ_{033}. If our samples differed substantially in the mean radius of the cylindrical lattice, the correlation coefficient would be large, because the changes in ξ's of 011 and 033 reflexions caused by different curvature of the lattice are mutually dependent. In our case, we found $r=0{\cdot}35$, which is a rather low value. We must, therefore, conclude that the samples do not differ substantially in the mean diameter of the cylindrical lattice. In TF1 we introduced the percentage deviation defined as $100(\xi_{cyl}-\xi_\infty)/\xi_\infty$, where ξ_{cyl} and ξ_∞ are the positions of the reflexion for the cylindrical lattice of finite and infinite radius respectively. As the deviation rapidly decreases with the increasing of the radial reciprocal coordinate of the reflexion, we introduce only a minor error by taking $\xi_{060}/6$ instead of ξ_∞ in computing the percentage deviation of reflexion 011.

The mean percentage deviation of reflexion 011 found for our fibres is 4·9%; the individual values have the standard deviation 0·7%. This corresponds to the mean diameter 280 Å if we suppose complete cylinders; and if we assume the presence of 8 planar boundaries in our samples (the incomplete cylindrical lattice with azimuthal extension $\pi/4$), we get the mean diameter 234 Å (see Fig. 8(*a*) and (*b*) in TF1). The corresponding standard deviations of individual diameters in our set of samples are 50 and 35 Å respectively. The value 234 Å is slightly larger than the 180 Å indicated by Whittaker (1957) as the most probable value of the diameter of the cylindrical lattice in his samples. Jagodzinski (1961) indicates the values of the inner radius and of the wall thickness for samples from New York and Thetford, from which one gets mean diameters of 174 Å and 240 Å respectively.

The width of reflexions

We measured the width at half maximum height. Even with a very well aligned sample the measured values were not identical for different orientations of the sample around the fibre axis; they fluctuated within $\pm 0{\cdot}001$ Å^{-1}. Results of the width measurements are summarized in Table 5.

The *h*0*l* reflexions are symmetrical and mostly narrow. No difference in width between reflexions 200 and 400 was found when the width was expressed in Å^{-1}. The mean values of the width of all reflexions are averaged over all the samples examined in this work, and the r.m.s. deviations of the measurements are shown in Table 6.

The r.m.s. deviation of the width of reflexions 200, 400 and 600 corresponds to the estimated reproducibility of the measurement of the width. For this reason we do not consider the differences in the width of the 200 and 400 shown in Table 5 as significant. We conclude, therefore, that the overall wall thickness, which can be deduced from the widths of the 200 and 400 reflexions is, within the limits of error of our observations, the same for all our samples. Assuming that the previously mentioned width of the 200 reflexion of the annealed copper wire can be considered as the measure

Table 4. *The r.m.s. deviations of radial reciprocal coordinates of measured reflexions for* 10 *independent measurements on fibre no.* 6

	Uncorrected					Corrected using K				
	200	400	060	011	033	200	400	060	011	033
$10^4\sigma_\zeta$	2·9	3·0	6·2	5·1	11·5	2·3	—	5·2	7·5	12·8

Table 5. *The half-height width* (Å^{-1}) *of measured reflexions*

Sample No.	200	400	202	060	011	033
1	0·006	0·006	0·009	0·014	0·012	0·018
2	0·006	0·006	0·008	0·015	0·013	0·017
3	0·007	0·008	0·014	0·014	0·017	0·021
4	0·007	0·007	0·016	0·014	0·020	0·025
5	0·007	0·007	0·009	0·014	0·013	0·018
6	0·007	0·006	0·007	0·013	0·017	0·019
7	0·007	0·007	0·006	0·014	0·013	0·017
8	0·008	0·008	0·009	0·015	0·013	0·020
9	0·006	0·006	0·011	0·015	0·016	0·022
10	0·006	0·006	0·019	0·015	0·019	0·028
11	0·007	0·007	0·010	0·016	0·015	0·022
12	0·008	0·009	0·008	0·014	0·019	0·018
13	0·009	0·009	0·016	0·016	0·018	0·019
14	0·007	0·007	0·008	0·015	0·012	0·014
15	0·007	0·007	0·007	0·015	0·015	0·020

of the instrumental broadening, and that both the profiles are approximately Gaussian, then the corrected mean value of the width of the 200 reflexion of the chrysotile is $6{\cdot}1 \times 10^{-5}$ Å^{-1}, and we get for the average value of the overall wall thickness 155 Å, which is in very good agreement with the 150 Å value given by Whittaker (1957).

The results of the measurement of the width of the 202 reflexion are more interesting. As can be seen from Table 6, the r.m.s. deviation is larger here than could have been expected on the basis of the inaccuracy of our measurement, and the mean value is also significantly larger. From Table 5 we observe that the width of reflexion 202 extends approximately from the width of the 200 reflexion to three times this value. This can be explained by the presence of some kind of axial disorder, probably by the presence of cylindrical axial boundaries occurring in our samples in different proportions. In Table 7, N_c, the mean number of these boundaries per elementary fibre is shown for individual samples.

Now let us examine the width of the 0*kl*-type reflexions. These reflexions, as shown in TF1, belong to the group with important contributions of high-order Bessel functions. Here, the equatorial reflexion 060 has, as have the equatorial reflexions of the *h*0*l* group, a rather small scattering of values of half-height width compared with reflexions of the same group on higher layer lines. r.m.s. deviation of the width of the 060 reflexion is presumably given by errors of measurement and alignment, so that we can accept the fact that the width of this reflexion is the same for all samples of our set, with a mean value of $14{\cdot}6 \times 10^{-3}$ Å^{-1}.

As was shown in TF1, the width of reflexion 060 is determined partly by the radius of curvature of the cylindrical lattice, and partly by the presence of planar boundaries. In the case of the absence of planar boundaries (complete cylindrical crystal), it follows from our computations that the widths of reflexion 060 are $15{\cdot}5 \times 10^{-3}$ and $14{\cdot}0 \times 10^{-3}$ Å^{-1} for the cylindrical lattice with mean diameters of 230 and 270 Å respectively.

Our measured value of $14{\cdot}6 \times 10^{-3}$ Å^{-1} can therefore be accepted as corresponding to the model of a cylindrical crystal with a mean diameter of about 250 Å, without planar boundaries at all or with planar axial boundaries only, which have no influence on equatorial reflexions. The mean-diameter value of about 250 Å is supported by our previous observation of the shift of the 011 reflexion as described above (see *The position of reflexions*).

Reflexion 011 is most important for the determination of the number of planar boundaries, because for this reflexion we computed (see TF1) the width as a function of the mean diameter of the cylindrical lattice, not only for the complete cylindrical lattice but also for different incomplete lattices. In Table 7 we show N_p, the number of planar axial boundaries, deduced on the assumption that the mean diameter is 270 Å; this diameter is one of the three for which the dependence of the width of the reflexions on the completeness of the cylindrical lattice was computed. The value is slightly larger than that found for our sample (see *The position of reflexions*) but it does not affect the general trend of N_p other than slightly increasing their values. If we compare N_c and N_p in Table 7, it is apparent that the numbers of cylindrical axial boundaries and planar axial boundaries are interdependent quantities. This is substantiated by the computation of the correlation coefficient r, which is 0·68 in this case.

The width of reflexion 033 on the third layer line depends, as does the width of 011, both on the curvature of the cylindrical lattice and on the number of planar misfit boundaries. Because of the large consumption of computing time when dealing with reflexions on incomplete cylindrical lattices having larger radial reciprocal coordinates, we did not compute the form of reflexion 033 in the same way as was done for the 011 reflexion. We computed only the dependence of the form of the 033 reflexion for a complete cylindrical lattice on the mean diameter, so that we cannot use the widths of 033 reflexions for the determination of the number of planar boundaries. From our computation it is seen that the width of the 033 reflexion is always larger than that of 011. For the complete cylindrical lattice with a mean diameter of 270 Å we found the widths $7{\cdot}7 \times 10^{-3}$ Å^{-1} and $10{\cdot}0 \times 10^{-3}$ Å^{-1} for reflexions 011 and 033 respectively. Further, if the different half-height width of 011 reflexions from different samples is caused by the different number of planar misfit boundaries in these

Table 6. *Mean width of measured reflexions* (Å^{-1}) *and the r.m.s. deviations of individual measurements* (Å^{-1})

	200	400	202	060	011	033
Mean width, Å^{-1}	0·0070	0·0071	0·0103	0·0146	0·0151	0·0199
r.m.s. deviation, Å^{-1}	0·0008	0·0010	0·0018	0·0008	0·0025	0·0032

Table 7. *The number of cylindrical* (N_c) *and planar* (N_p) *axial boundaries*

Sample No.	N_c	N_p	Sample No.	N_c	N_p	Sample No.	N_c	N_p
1	0·5	8·5	6	0·1	13·4	11	0·4	11·8
2	0·3	9·4	7	0·0	9·4	12	0·0	10·6
3	0·5	13·4	8	0·1	9·4	13	0·8	15·2
4	1·3	17·0	9	0·8	12·7	14	0·1	8·5
5	0·3	9·4	10	2·2	16·0	15	0·0	11·8

samples, then the width of the 033 reflexion must have the same trend. The correlation coefficient $r=0{\cdot}79$ for the width of the 011 and 033 reflexions confirms this to a large degree.

Conclusions

From our measurements of the form, position and half-height widths of reflexions from chrysotile asbestos fibres of different origins, the following results are shown:

1. Within the limits of error there is no difference in the wall thickness and the mean diameter of the cylindrical lattice among our 15 samples. The average wall thickness was found to be 155 ± 1 Å, and the average mean diameter less than 280 ± 2 Å, probably about 234 ± 1 Å. (Confidence limits are equal to the estimated values of the r.m.s. deviation of averages.)

2. From the form of reflexion there is strong evidence in favor of Whittaker's model of distribution of cylindrical azimuthal boundaries separating silica–brucite double layers. However, the form of reflexion 031 suggests that there may be a reason for considering a model with less than the maximum number of cylindrical azimuthal boundaries per elementary fibre, perhaps similar to the one dealt with in TF1, Fig. 5(*b*).

3. The most interesting feature is the presence of axial disorder which causes the equatorial reflexion of both *h*0*l* and 0*kl* types to display larger 'particle size' than the higher layer line reflexions. There is an indication of a correlation in the number of the cylindrical axial boundaries and the planar axial boundaries in our samples. We believe that the dark radial lines on the electron micrographs in the paper of Maser, Rice & Klug (1960), Figs. 2(*c*) and 3, confirm our finding of the presence of planar boundaries.

4. We could find no apparent close correlation between tensile strength and type or number of misfit boundaries, which suggests that interfibre binding may be an important factor in tensile strength.

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On the Information about Deformations of the Atoms in X-ray Diffraction Data

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The information which can be obtained about the shape of crystal atoms by X-ray diffraction is studied in light of a model calculation. The electron density of an atom is treated as a Fourier invariant expansion in terms of harmonic oscillator wave functions adapted to the crystal symmetry. Definite limits for the observability of the terms are set by the experimental cutoff in $\sin\theta/\lambda$, and by the volume of the atom. As a consequence, details smaller than a critical size cannot be seen either in the electron density or in the atomic factor. Experimental errors are such that the atomic factor rather than the electron density reveals the significant deformations. Termination effects are studied in a model crystal: deformations are inserted and a truncated set of structure amplitudes is analysed. Here series were used for the radial coefficients ϱ_l, f_l in the harmonic expansions $\Sigma\varrho_l(r)_l K(\theta,\varphi)$ and $\Sigma f_l(b)K_l(\theta,\varphi)$ for the electron density and the scattering factor of a sphere. The radial scattering factors are well reproduced up to the cutoff value of the reciprocal vector, while a fair representation of the radial densities can be reached only by a long series. The termination does not significantly mix components with different angular behaviour. Reasonable contributions from neighbouring atoms have no major effect on the radial scattering factors or densities. Therefore the factors f_l calculated for a slightly 'too large' sphere will lead to a proper interpretation of the electron distribution in terms of deformed atoms.

1. Introduction

The concept of atomic deformation refers to the idea that we are analysing the structure of the crystal in terms of separate atoms. Actually it is surprising how well the separate atom model works in spite of the interactions between the atomic electrons in the solid state. Still to day almost all experimental diffraction data on crystals can be explained by models built from free atoms vibrating about their lattice sites. Only recent