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Correction of integrated x-ray intensities for preferred orientation in hexagonal close-packed powders

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Abstract

The symmetrized harmonic method of correcting integrated x-ray intensities for preferred orientation in powder samples is extended to hexagonal close-packed crystals. The method is based on the measurement of the intensity variation of a few reflexions in a limited range of polar angle. This information fixes the first few terms in the harmonic expansion describing the orientation distribution of crystallites, which is sufficient to provide reliable corrections for all reflexions. Model calculations showed that the reliability of the corrections depends strongly on the combination of reflexions used. Three properly chosen reflexions already produce the attainable accuracy even in the presence of small granularity effects. In the case of a regular orientation, omission of high order terms in the harmonic expansion improves the overall accuracy of the corrections. The method was tested experimentally on four magnesium samp'es with different degrees of orientation, the largest correction being 76 %. Two independent checks were made. First, the relative intensities of six reflexions were measured from each sample separately and, secondly, the same reflexions were measured one at a time from all samples in equivalent conditions. The consistency of the results indicated that the accuracy of the final intensities after correction was about one per cent.

1. Introduction

X-ray intensity measurements from powder samples are a standard technique in charge distribution studies of crystalline matter. Its practical use is, however, limited by the fact that very accurate intensities are required for the observation of solid state effects. During the last decade the experimental technique has improved to the stage where different sample effects dominate the residual inaccuracy. Many factors such as porosity, surface roughness, inhomogeneity of packing and preferred orientation cause significant systematic deviations of the actual intensities from those of an ideal powder sample.

It has been found from experience that the effect of preferred orientation is in general stronger when heavier stress is used in the sample preparation. Therefore

light pressure and even loose packing have been attempted so as to minimize the effect. This, in turn noticeably increases surface roughness, porosity and inhomogeneity effects. Moreover, even this technique does not assure complete disappearance of the orientation effect. To the contrary, a coupling to the other sample effects makes the orientation irregular and therefore difficult to control. Another possibility for minimizing the total error is to seek experimental conditions under which the other sample effects would be less significant, while the orientation would be well formed and regular so that one could estimate its total effect with reasonable accuracy and then correct for it. This requires the use of sufficiently hard-pressed specimens.

Järvinen *et al.* [1] showed that, at least in favourable cases, the orientation errors in integrated intensities can be corrected to an accuracy comparable with the errors associated with experimental procedures in intensity measurements. The determination of the corrections is based on the assumption that in case of a well formed, but not too strong, orientation the orientation distribution of the crystallites can be represented with fair accuracy by the first few terms of its expansion in properly symmetrized harmonics. The experimental information required for evaluation of this expansion and for subsequent estimation of corrections can be obtained by measuring the integrated x-ray intensities of a few reflexions for various tilting angles of the specimen.

Järvinen *et al.* [1] presented the general theoretical principles of the method, but so far the only application has been to cubic powders. The object of this paper is to study the applicability of the method to hexagonal close-packed crystals and so to obtain a further independent test of its general principles. In particular, it is important to establish just how much experimental information will be necessary to obtain a reliable picture of the orientation effect. The possibilities of arranging experimental conditions corresponding to the assumptions of the method depend strongly on the properties of the material studied. Magnesium turns out to be a suitable material. First, a powder of spherically shaped particles with ideal packing properties was available, which made it easier to prepare homogeneous samples with a regular but not too strong orientation. Secondly, its low absorption results in effective reduction of inaccuracies arising from surface properties and inhomogeneities in the specimen.

2. Theory

The orientation distribution of the crystallites in a powder specimen is defined by the polar axis density

$$W(\vartheta, \varphi) = \frac{4\pi \, \mathrm{d}V}{V_0 \, \mathrm{d}\Omega} .$$

Here V_0 is the total volume of the crystallites in the specimen and dV is the volume occupied by those crystallites with such an orientation that the surface normal

of the specimen falls within a solid angle element $d\Omega$ in the direction ϑ, φ with respect to the internal crystallographic axes. In an ideal sample the orientation distribution is completely random, corresponding to $W(\vartheta, \varphi) \equiv 1$. The diffracted intensity is proportional to the scattering volume and hence to the polar axis density in the relevant direction ϑ, φ. Generally this direction makes an angle α, the polar angle, with the scattering vector. In the conventional measuring geometry we have $\alpha = 0$ and the observed intensity I^{hkl}_{meas} is proportional to $W(\vartheta_{hkl}, \varphi_{hkl})$. Therefore

$$I^{hkl} = I^{hkl}_{\text{meas}} / W(\vartheta_{hkl}, \varphi_{hkl}) \tag{1}$$

represents intensities corrected for nonuniform orientation distribution.

The polar axis density will always possess the symmetry of the crystal structure. It can therefore be represented by the expansion

$$W(\vartheta, \varphi) = \sum_{ij} C_{ij} K_{ij}(\vartheta, \varphi) \tag{2}$$

in terms of harmonics K_{ij} symmetrized with respect to the relevant point-group symmetry. It is practical to use two indices; i denotes the order of the harmonics while j labels the independent harmonics within each order. Since $W(\vartheta, \varphi)$ by its physical nature is an even function, the index i runs through even values only. The mean value of $W(\vartheta, \varphi)$ is $C_{00}K_{00} = 1$, by definition. Determination of the other coefficients C_{ij} from the experimental information is the main problem to be solved. When the specimen is spun about the surface normal, the observed intensity will be proportional to the corresponding average of $W(\vartheta, \varphi)$. Integration of eq. (2) gives the Legendre polynomial expansion

$$I^{hkl}_{\text{meas}}(\alpha) = \sum_{i} b^{hkl}_{i} P_i(\cos\alpha) \tag{3}$$

for the integrated intensity of the reflexion hkl at polar angle α. The coefficients are given by

$$b^{hkl}_{i} = T^{hkl} \sum_{j} C_{ij} K_{ij}(\vartheta_{hkl}, \varphi_{hkl}) \tag{4}$$

where T^{hkl}_{i} is a necessary proportionality constant.

This shows, in principle, the relation of the unknown coefficients to the intensity measurement for various tiltings α of the specimen, and thus forms the basis of the treatment of our problem. In the case of hexagonal close-packed crystals the symmetrized harmonics K_{ij} are readily found by direct symmetrization of the spherical harmonics $Y^m_i(\vartheta, \varphi) = P^m_i(\cos\vartheta)e^{im\varphi}$. The relevant symmetry operations are:

1. A 60° rotation around the z-axis: For $m = 6j$ with integer j Y^m_i is invariant. In all other cases the symmetrization yields zero.

2. Reflexion through the xy-plane normal to the z-axis: Y^m_i is invariant for $(i-m)$ even. All other harmonics vanish under symmetrization.

3. Reflexion through the xz-plane parallel to the z-axis: If we choose the x-axis to be in this plane, each pair $e^{\pm im\varphi}$ yields cos $m\varphi$ under symmetrization.

When applied simultaneously these three symmetrizations lead to the hexagonal symmetrized harmonics

$$K_{ij}(\vartheta, \varphi) = A_{ij} P_i^{6j} (\cos \vartheta) \cos 6j\varphi; \; i = 0, 2, 4 \ldots, 6j \leq i \tag{5}$$

where the A_{ij} will be chosen to fulfill the practical normalization condition max $|K_{ij}| = 1$ introduced by Kurki-Suonio and Ruuskanen [2].

The limitation to a regular and not too strong orientation indicates that high order terms in the series (2) and (3) will be negligible. By analogy to the cubic case treated by Järvinen *et al.* [1] we omit all terms with $i > 10$. Even with this limitation we have nine different functions

$$\begin{aligned} K_{i0} &= P_i (\cos \vartheta); \; i = 0, 2, 4, 6, 8, 10 \\ K_{61} &= \sin^6 \vartheta \cos 6\varphi \\ K_{81} &= \frac{2000}{2401} (15 \cos^2 \vartheta - 1) K_{61} \\ K_{10,1} &= 0.24242 \, (323 \cos^4 \vartheta - 102 \cos^2 \vartheta + 3) K_{61} \end{aligned} \tag{6}$$

Correspondingly, there are eight parameters C_{ij} to be evaluated. In addition, fitting of series (3) to experimental information involves T^{hkl} as extra parameters.

Accurate knowledge of $I^{hkl}(\alpha)$ for the reflexion hkl would give directly all coefficients b_i^{hkl}. Thus, in principle, information about one reflexion hkl would suffice to determine C_{20} and C_{40}, while study of at least two non-equivalent reflexions is necessary to obtain the two coefficients C_{ij} in each of the orders $i = 6, 8, 10$.

The accuracy of C_{ij} obtained from the measurement of a certain reflexion hkl obviously depends on the values $K_{ij}(\vartheta_{hkl}, \varphi_{hkl})$; in the limiting case where $K_{ij} \ll 1$ the reflexion does not contain any information about C_{ij}. Table I, which gives values of hexagonal harmonics for the first six reflexions of magnesium, thus gives an idea of the usefulness of different reflexions from this point of view. The reflexion 002 is clearly the most favourable one for determination of the first two nonspherical terms, which are the most important ones. The next best is 100 or 110, while the smallness of both K_{20} and K_{40} makes 101 somewhat more ineffective, and 103 will give practically no information on C_{40}. The reflexion 002 can equally well be used to estimate the higher order ($i = 6, 8, 10$) coefficients C_{i0}, while it gives no information about C_{i1}. On the other hand, the coefficients C_{i1} dominate the higher order behaviour of the reflexions 100 and 110, which with their different signs for K_{i1} form a suitable pair for studies of C_{i1}, if desired.

From the general properties of orthogonal series we know that details in the behaviour of $I^{hkl}(\alpha)$ do not affect the low order terms of expansion (3). This means that, for determination of the coefficients b_i^{hkl} up to the 10$^{\text{th}}$ order, information at intervals of about 10 degrees in α will be sufficient. Moreover, measurement at

Table I. Values of hexagonal harmonics for the first six reflexions of magnesium.

hkl	$\cos\vartheta$	φ	K_{20}	K_{40}	K_{60}	K_{61}	K_{80}	K_{81}	$K_{10,0}$	$K_{10,1}$
100	0	0°	−0.5	0.375	−0.3125	1	0.2734	−0.8330	−0.2461	0.7273
002	1	—	1	1	1	0	1	0	1	0
101	0.4706	0°	−0.1677	−0.2410	0.3321	0.4718	−0.1495	0.9128	−0.1114	−0.4284
102	0.7296	0°	0.2985	−0.3815	−0.2201	0.1023	0.2563	0.5952	0.2016	0.9976
110	0	30°	−0.5	0.375	−0.3125	−1	0.2734	0.8330	−0.2461	−0.7273
103	0.8480	0°	0.5787	−0.0591	−0.4053	0.0221	−0.2618	0.1806	0.1151	0.5192

shorter intervals does not produce essentially more independent information, its significance being only a statistical improvement.

On account of the measuring geometry the effective region of measurements ranges up to about $\alpha = \pm 60°$. Only around half of the orthogonality interval of the Legendre polynomials in $\cos\alpha$ is thus covered. This is a severe limitation. The complete independence of the terms of series (3) due to orthogonality is lost (and consequently the uniqueness of the representation) which leads to reduction in the accuracy of the coefficients. This disadvantage will be partly cancelled by use of more reflexions. There is another reason why the theoretical minimum number of reflexions is not sufficient in practice. The numerous and complicated potential sources of error result in effects which are specific in any single piece of data, but which can be treated as statistical effects when a large set of independent data are treated simultaneously. Therefore we must keep track of two kinds of statistics. Good statistics on each value measured is necessary, but in addition the amount of independent data available must also be statistically significant compared with the number of parameters to be determined. Measuring an α range of 60° at intervals of 10° requires at least three different reflexions to obtain a statistically meaningful set of independent data for fixing all the parameters involved. This situation does not depend appreciably on the number of terms treated. If, for instance, we include only the most important low-order terms $i \leq 4$, we have just two parameters C_{i0} (plus T^{hkl}), but, correspondingly, now we do not get statistically independent information on them at smaller intervals than about 20°.

The treatment of experimental data as well as the model calculations were arranged to investigate the significance of these qualitative considerations more quantitatively.

3. Model calculations

To analyse the effect of different factors on the reliability of the method a series of calculations were performed. An orientation model was defined by giving fixed numerical values to the coefficients $C_{ij} (i \leq 10)$ of the polar axis density (2). These were chosen to correspond to the observed coefficients of one of our samples with stronger orientation effects (specimen D). Numerous sets of model data $I^{hkl}_{\text{meas}}(\alpha)$ corresponding to different ways of collecting data were generated by adding random errors to the exact model values. These »data» were then used to recalculate the coefficients C_{ij} and the orientation corrections $W(\vartheta_{hkl}, \varphi_{hkl})$ for the first six reflexions. The degree of fit with the original values then served as a measure of the reliability.

Particular attention was paid to the following points:

1. differences in the reliability when different reflexions and different combinations of reflexions are used;
2. reduction of information due to the limited range of polar angle, and particularly

the possibilities of replacing this reduction by use of more reflexions;
3. significance of the interval $\Delta\alpha$;
4. importance of the statistical quality of the data, i.e. the accuracy and the total number of observed values; and
5. the effect of the length of series (2) on the necessary qualifications of data.

First, the terms with $i \leq 4$ only were included in the analysis. To study points 1 to 3, data with equal statistical quality for different combinations of reflexions and for different α ranges and intervals were generated by keeping the »experimental errors» at the level of one half per cent and by using a fixed total number of data. Point 4 was studied by making similar calculations at the one per cent error level and by varying the total number of data. Finally, point 5 was studied repeating the model analysis with terms up to $i = 10$.

The short series calculations showed clearly that full range ($\alpha_{max} = 90°$) data on one reflexion is sufficient to give the coefficients C_{20} and C_{40} reliably within the accuracy provided by the data. In this respect minor differences between different reflexions could be observed. In the case of a realistic α range ($\alpha_{max} = 60°$) one reflexion was not enough and different combinations of reflexions differed considerably from each other in reliability. The pair 100,002 was clearly the most favourable one. However, three reflexions at least, preferably with this pair included, seemed to be necessary to replace the loss of information due to the reduced α range. With these conditions the deviations in the results were already comparable to the »experimental errors» and a further addition of reflexions gave no improvement. Further reduction of the range to $\alpha_{max} = 50°$ or even 40° turned out to be possible if the statistical quality of the data was kept at the same or a higher level. The role of the interval $\Delta\alpha$ seemed unessential as compared with the effect of the statistical quality of the data. Thus $\Delta\alpha = 10°$ seemed to be sufficiently dense in all cases, while careful measurement of the $I^{hkl}(\alpha)$ values is obviously important. Data on three favourable reflexions with good statistics yielded essentially better results than data of lesser quality on five or six reflexions.

Analysis with longer series in the main merely confirmed the above results. However, the larger number of parameters seemed to put more stringent requirements on the data. Although, in principle, two reflexions are sufficient in the case of a full α range, good results were obtained at the statistical quality used only when at least three reflexions were used. In the case of three or four favourable reflexions the α range could be reduced to $\alpha_{max} = 60°$, but the results were substiantally worse than those calculated with $i \leq 4$ and using the same data. Shorter ranges, $\alpha_{max} = 50°$ (and 40°), seemed to require very high quality data and the combination of at least four favourable reflexions.

The surface roughness is expected to cause the greatest systematic errors in the behaviour of $I^{hkl}(\alpha)$. This leads typically to a monotonous reduction of $I^{hkl}_{meas}(\alpha)$ as a function of polar angle. To examine its effect on the reliability of the orientation corrections we made further model calculations in which the data, with no

random errors, ranged up to $\alpha_{max} = 40°$, 50° or 60°. From the general behaviour of the surface roughness effect [3] the reduction of I^{hkl} (60°) was estimated as 0.8 and 2.3 per cent for two different cases, respectively. The results of the model calculations tended to favour the use of shorter α ranges. Moreover, the inclusion of the reflexions 100 and 002 turned out to be essential. Here again shorter series gave better results: The average deviation in the W values obtained in favourable fittings were about 0.1 and 0.4 per cent for terms with $i \leq 4$, while the corresponding values with $i \leq 10$ were 0.2 and 0.8 per cent, respectively, for the two above mentioned reductions in $I^{hkl}(\alpha)$.

4. Experimental results

The system for measuring the distribution $I^{hkl}(\alpha)$ was composed of the usual Siemens diffractometry equipment and texture goniometer, which made possible α rotation and specimen spinning. The reflexion method used was originally proposed by Schulz [4]. Here the symmetrical horizontal divergence of the primary beam was 0.8° and the vertical divergence was $\leq 1.3°$. The influence of increasing the vertical divergence from 0.6° to 1.3° was examined experimentally but no significant effect was found. The width of the receiving slit was $\Delta(2\theta) = 2°$ or 3° depending on the reflexion measured. The integrated intensity of the whole reflexion was measured at one time. We used nickel filtered Cu radiation.

The atomized magnesium powder investigated in these measurements was manufactured by K & K Laboratories. The average particle size reported was 18 μm. According to microscopic examination the particles were spherical. In spite of this we were unable to prepare a specimen free from orientation effects. Four test specimens (A, B, C and D) were made in a cylindrical holder using pressures of 100, 300, 500 and 700 kp. cm^{-2}, respectively. The surface of each sample was smooth. The intensity distributions $I^{hkl}(\alpha)$ of the reflexions 100, 002 and 101 were measured up to $\alpha = 60°$ at intervals of 10°; the reflexions 102, 110 and 103 were measured only for specimen D, for checking purposes. The differences between the two series of $I^{hkl}_{meas}(\alpha)$ values were about one per cent or less. The distribution $I^{hkl}_{meas}(\alpha)$ was symmetrized in order to minimize possible asymmetry effects of the primary beam.

The coefficients C_{ij} were determined by simultaneous least squares fitting of series (3) to the $I^{hkl}_{meas}(\alpha)$ values of the first three reflexions. The values obtained, corresponding to shorter ($i \leq 4$) and longer ($i \leq 10$) series, are shown in Table II. The orientation coefficients W of different reflexions were then calculated by eq. (2) and are listed in Table III. Their reliability was examined as follows. The relative integrated intensities of the first six reflexions for each specimen were measured by the standard scanning method and using the primary beam monochromator technique. The intensity series, corrected for preferred orientation, were then put onto the same scale by the method of least squares. For each reflexion the deviations δ_1 from the mean intensity value are presented in Table III. In addition, the

Table II. The coefficients C_{ij} of specimens A, B, C and D determined by simultaneous least squares fitting of series (3) with a) $i \leq 4$ b) $i \leq 10$ to the I^{hkl}_{meas} (α) values of the reflexions 100, 002 and 101.

	a)			b)								
	C_{00}	C_{20}	C_{40}	C_{00}	C_{20}	C_{40}	C_{60}	C_{61}	C_{80}	C_{81}	$C_{10,0}$	$C_{10,1}$
A	1	0.031	0.022	1	0.034	0.008	− 0.004	0.005	0.027	0.005	0.007	0.004
B	1	0.231	0.026	1	0.240	0.023	−0.010	0.006	0.019	0.004	− 0.013	−0.001
C	1	0.440	0.074	1	0.436	0.068	−0.005	0.011	−0.009	0.006	0.036	0.009
D	1	0.671	0.087	1	0.667	0.093	− 0.014	0.005	0.012	0.014	0.002	−0.009

Table III. The values W of specimens A, B, C and D corresponding to the coefficients C_{ij} in Table II. δ_1 are the residual percentage deviations from the mean value of the normalized relative intensities and δ_2 are the respective deviations when each reflexion was measured separately under identical conditions.

	hkl	W_A	δ_{1A}	δ_{2A}	W_B	δ_{1B}	δ_{2B}	W_C	δ_{1C}	δ_{2C}	W_D	δ_{1D}	δ_{2D}
	100	0.993	0.4	− 0.1	0.894	0.0	− 0.1	0.808	0.2	0.6	0.697	−0.6	−0.4
	002	1.052	−0.5	−0.3	1.257	−0.3	− 0.4	1.515	1.1	1.9	1.759	− 0.2	−1.2
	101	0.990	−0.1	−0.4	0.955	− 1.3	−1.0	0.908	0.5	0.5	0.866	1.0	0.9
a)	102	1.001	0.5	0.5	1.059	− 0.8	−0.7	1.103	0.6	0.7	1.167	−0.2	−0.5
	110	0.993	−1.0	−1.7	0.894	0.8	1.2	0.808	− 1.1	−0.6	0.697	1.1	1.1
	103	1.017	0.8	0.9	1.132	1.6	1.2	1.250	− 1.4	− 0.8	1.383	− 1.1	−1.3
	100	0.997	0.4	−0.2	0.903	− 0.7	− 0.7	0.810	0.0	0.6	0.694	0.3	0.3
	002	1.072	−1.5	−1.4	1.259	0.1	0.1	1.526	0.8	1.9	1.760	0.6	−0.6
	101	0.991	0.4	0.0	0.956	−1.0	−0.6	0.913	0.2	0.5	0.878	0.4	0.1
b)	102	1.024	−0.3	− 0.4	1.069	−0.6	−0.3	1.124	−0.2	0.1	1.170	1.1	0.6
	110	0.989	−0.2	− 1.1	0.897	0.6	1.0	0.786	1.5	2.3	0.722	−1.9	−2.2
	103	1.018	1.2	1.1	1.136	1.5	1.2	1.263	−2.3	−1.5	1.382	−0.4	−0.8

integrated intensities from the specimens were measured under identical conditions for each reflexion separately. In this test we applied Suortti's method [3] for determining the corrections for the porosity effect, which were found to be ≤ 1.7 per cent. The deviations δ_2 of the corrected intensities from the corresponding mean values are shown in Table III. The uncertainty of the measured intensities was estimated to be less than one per cent except for the 103 reflexion, where it was larger owing to difficulties in background subtraction.

5. Conclusions

Table III shows good consistency of the integrated intensities corrected for preferred orientation and porosity effects. The two independent checks for the intensities give additional opportunity to estimate the statistical accuracy of the intensity measurements; this is seen to be of the order of half a per cent. Further examination shows that the deviations δ_1 and δ_2 are correlated. This effect must be due to deviations of the true orientation distributions from the low order harmonic model and to variations in the samples in this respect. These systematic errors are, however, very small and it seems clear that the method for correcting for preferred orientation effects described by Järvinen *et al.* [1] is applicable also to hexagonal close-packed crystal powders.

High statistical accuracy of the $I^{hkl}_{\mathrm{meas}}(\alpha)$ values is a necessary condition for reliable corrections. The only way to realize this in a reasonable time appears to be the use of a broad receiving slit so that the whole reflexion is measured at one time.

The assumption of regular orientation distribution in the sample can usually be fulfilled by preparing the specimen with sufficient care. The powder must be fine grained and homogeneous, and it must be packed in homogeneous thin layers without shaking the moulding die. A relatively high pressure in preparing the specimen is recommended. In this way inhomogeneities created in the packing process will be largely smoothed out. Irregularities in the orientation distribution are revealed through exceptionally large residual differences $I^{hkl}_{\mathrm{meas}}(\alpha) - I^{hkl}_{\mathrm{fit}}(\alpha)$ or, especially if only a few reflexions are used, through some large high order coefficients C_{ij}. Such samples are inadequate for accurate intensity measurements.

Use of a specimen spinner in ordinary intensity measurements effects the averaging of the intensity around a circle. Through this symmetrization the effects of irregularities of the sample are to a certain extent further smoothed out. It is naturally important to use the same procedure also in the $I^{hkl}(\alpha)$ measurement. This largely explains why the $I^{hkl}_{\mathrm{meas}}(\alpha)$ distributions turn out to be so smooth that even relatively strong orientation effects can be represented by the low order harmonic model to sufficient accuracy. Without spinning so much more information would be needed that it would become practically impossible to solve the problem. Both the model calculations and the experimental results show that the inclusion of high order terms increases the influence of statistical and systematic errors on

the corrections. Limitation to low order terms, up to fourth order in the present case, is therefore not only justified but leads to a more reliable overall correction of the preferred orientation, as observed.

The errors arising from measuring geometry and surface roughness increase with the tilting angle and limit the useful α range to fifty or sixty degrees. This disadvantage can be cancelled somewhat in the analysis by combining data from several reflexions. If the reflexions 100 and 002 are among those measured, three reflexions seem to give a satisfactory result. In this study the surface roughness effect was not discernible, and increasing the number of reflexions from three to six did not improve the consistency of the results.

The orientation effect is much stronger in magnesium than in aluminum powders studied by Järvinen *et al.* [1]. We did not succeed in preparing a specimen without appreciable orientation. This is not surprising because of the difference in the symmetry. Thus if the powder method is used to study the detailed behaviour of the electron density in hexagonal or other strongly axial crystals, the effect of preferred orientation must be corrected for in every sample before any reasonable conclusions can be made. In this study the correction of intensities for preferred orientation succeeded to the extent of an error of about one per cent in the final intensity. This is already a sufficient accuracy for very detailed analysis. Generally speaking, the method offers a possibility for quantitative examination and correction of the orientation effect and places the discussion of accurate x-ray intensity measurements on a more reliable level.

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